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P O W D E R
S U I T E

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Chapter 1: OVERVIEW

The Powder Suite package of computer programs is designed for interactive and limited batch processing of powder diffraction data. The package consists of several programs, which are briefly discussed in this chapter, and in more detail in a chapter devoted to each program. Also discussed here are features that are used all programs.

1.1 Organization of Programs

The programs used in this package all have the same type of internal organization, modeled after the command structure of the VAX/VMS DCL command language. Once the program is started, any appropriate command for that program may be entered, usually in any sequence. The format for a command is:

```
COMMAND[/qualifiers] [parameters]
```

or

```
COMMAND [parameters][/qualifiers]
```

(the `[ ]` symbols are used to indicate that an option need not be specified.) If it is desired to spread a command over several lines, end all but the last line with a dash (`-`).

For most commands, it is possible to achieve the same results by specifying command with no qualifiers or parameters and the program will prompt for important options (prompt – meaning the computer will request input). It is often faster to specify options on the command line. However, some infrequently used options on certain commands are only available on the command line.

For example, in program CMPR, a file may be plotted by typing

```
PLOT
```

this causes the program to prompt for file number(s) and some scaling information. Typing

```
PLOT 1/XLOW=10/XHIGH=40
```

Causes file 1 to be plotted from 10 to 40 degrees. The `/TITLE` option, which puts the file's title on the plot can only be requested with a qualifier. To get a title on a plot type one must enter

`PLOT/TITLE` or

```
PLOT 1/XLOW=10/XHIGH=40/TITLE
```

Programs which offer a `DEFAULT` command have two modes AUTO and MANUAL. In AUTO mode the program will use default values for options wherever possible. However, if an option is specified on a command line, the command line specification overrides the default.

At this time, not all options within a command may be specified on the same line as a command, but this will be changed in later versions of the package to allow those commands to be used in batch mode.

1.2 Description of Programs

A brief description of the programs currently contained in the package follows. Complete documentation of the commands available in each program may be found in a following chapters.

1.2.1 Program LOGIC

Program LOGIC locates entries in the JCPDS-ICDD data base either from a JCPDS-ICDD entry number or by searching the database for compounds matching a specified chemical composition, chemical/mineral name or with peaks in selected regions. The program can display or print relative intensities versus 2θ or d-spacings for the selected entries, or plot the same data, optionally displaying an experimentally determined powder diffraction pattern or set of peaks on the same scale. LOGIC may also be used to examine lists of matching patterns determined by program SEARCH. Experimentally determined peak positions may be read from the SEARCH parameter file for graphic display along with the matching patterns.

1.2.2 Program SEARCH

Program SEARCH is used to search the JCPDS-ICDD database to identify unknown phases in patterns. Peaks may be input directly to SEARCH, or can be read from a data file written by MANIP. Chemistry requirements may be used to limit the number of entries that must be examined by using the LOGIC program, which may be called from within SEARCH. Use of chemistry also reduces the number of spurious matching patterns by eliminate from consideration materials with unlikely compositions. Depending on the number of entries to be examined, the database search may require anywhere from seconds to several minutes of computer time, so the user has been given the option to execute the search either interactively, or with a batch job – freeing the terminal for other uses. SEARCH writes a file of parameters which may be reread and modified in a later SEARCH run.

1.2.3 Program CMPR

Program CMPR is used for comparison of diffractograms. Data may be plotted, added, subtracted, and/or compared to JCPDS-ICDD entries. This program is still under development.

1.2.4 Program MANIP

Program MANIP is used for processing of a single diffractogram. Operations that may be performed include baseline assignment and stripping, $K\alpha_2$ stripping, interpolation, smoothing and peak processing. This program is still under development.

1.2.5 Program ENCODE

Program ENCODE is actually a sequence of four programs which create the files needed by Powder Suite from the full (PDF-2) JCPDS-ICDD database.

The first program, PDF1, reads the PDF-2 database and creates a condensed subset of the original database called the PDF-1 database. These entries may also be indexed by the PDF1 program and will be accessible by the other Powder Suite programs. Optionally users may add their own PDF-2 entries to the database using this program.

The second program, ADDPDF1, is used to add PDF-1 format entries to the PDF-1 files written by program PDF1. These entries are easier to prepare than PDF-2 entries. Use of this program is optional.

The third program, WRDI, is used to create the d-space index files which are used for rapid searching of the database by peak position.

The fourth program, WRCHEM, is used to create the elemental composition index files which are used for rapid searching of the database by chemistry.

1.3 DCL Command Procedure

The VAX/VMS operating system provides a subdirectory structure that allows users to catalog their datafiles by storing them in different subdirectories. While fully-specified file names may be input for file names to the Powder Suite programs, it is usually most convienient to use the name without a device, directory and extension. In this case, most files will be written in the current default directory with an extension selected by the program. (Certain temporary files will be written in a designated scratch directory, `PS_TMP:`). It is suggested that users of these programs periodically "clean-up" (delete unneeded files from) their working and scratch directories. The clean-up process is easier if several subdirectories and descriptive file names are used so that junk may be discerned from still-needed information. If the user creates a subdirectory for each project and sets current default (using the DCL `SET DEFAULT` command, or the equivalent) to the appropriate subdirectory before using the PS package, all files for that project will be placed in that subdirectory.

To aid in using the Powder Suite package from a directory or disk other than where the programs are stored, a command procedure named `PS.COM` defines the required logical names and symbols. Typing

```
$ @dev:[dir.PS]PS
```

where `dev:[dir.PS]` is the location of the Powder Suite files, starts a menu where a user can access the programs or get help information. After the first time the procedure is called, a symbol `PS` is defined which is equivalent to the above command, so typing `PS` will also start the package. For convenience the symbol PS may be defined as

```
$ PS    :==   @dev:[dir]PS
```

in the user's or system login file and the user never needs to use the initial `@dev:[dir.PS]PS` command. (An alternative to this is to place the command

```
$ @dev:[dir]PS INIT num
```

in the user's `LOGIN.COM` file; this defines a terminal type as `num`, (see the Customization Instructions).

To run a specific command, it is possible to bypass the menu, by typing

```
$ PS command
```

for example, `PS LOGIC` or even `PS L` to start program LOGIC. Note that program names can be abbreviated down to any unique abbreviation (eg. `C` for CMPR).

The first time the `PS.COM` procedure is called, a second file, `PS_INIT.COM`, is also executed which defines all of the symbols and logical names required by the package. When the package is first installed, the `PS_INIT.COM` should be updated to reflect the local computer environment (device names etc.)

In addition each user can have one or more customized `PS_LOCALINIT.COM` files. The following locations are searched (in the order specified) for the `PS_LOCALINIT.COM` file:

(1) the current default directory

(2) the current login directory (as defined by `SYS$LOGIN`).

In this way, by placing `PS_LOCALINIT.COM` files in different locations, differing sets of logical names may be used by different users or even for different projects. The package may be reinitialized at any time by typing

```
PS INIT
```

The symbols and logical names defined in the PS_INIT.COM file are discussed in more detail in the Customization Instructions chapter at the end of this manual or in ASCII file CUSTOMIZE.DOC, which is distributed with the package.

The installation procedure can be used to create the PS.COM and PS_INIT.COM files with definitions suitable for the system where the programs have been installed. This is discussed in more detail in the Installation Instructions chapter at the end of this manual or in ASCII file 1README.1ST, which is distributed with the package.

1.4 On-line Help Information

The programs documented here all have VAX help files which may be accessed either from inside the program or directly from the PS.COM procedure using the HELP option. The help information is quite similar to the text of this manual.

From inside a program, type the HELP command to access the help menu. The options for which further information is available will be listed following help text. For example, inside program LOGIC, at the LOGIC> prompt, type HELP to access the help file. A list of commands will be displayed. Then type (for example) MATCH for information on the MATCH command. There are several sub-options within MATCH, which can then be examined. To return to the program press the control key and the Z key at the same time (this action is usually called a control-Z sequence and is will be abbreviated as ^Z).

From the PS.COM procedure, first type HELP and then ask for the specific help library by typing, for example, @LOGIC. From this point, help is available as described above.

1.5 Data and Peak File Formats

There are two types of data files recognized in the Powder Suite programs, data files and peak files. Data files usually contain the raw diffraction results and values describing how the measurement was made, while peak files contain derived results such as peak positions, heights and areas. Occasionally a single file may contain both sets of information.

The philosophy used in the Powder Suite programs is to allow the programs to read as many different types of data files as can be conveniently incorporated and to allow the programs to be easily expanded to accept additional formats. Also, rather than require users to specify the format of the file they want to read, the code has been written to automatically determine the format by reading the file.

Associated with each file format is a default extension. For example, DuPont files are expected to have extension .DDAT, and Brookhaven X7A files are expected to have extension .X7A. If a program is instructed to read data file TEST, then it will first search for a file named TEST.DDAT and if it is found check if it is in DuPont format, if no such file is found or the file cannot be read, it will then search for a file named TEST.X7A. Successive attempts will be made until each file type has been tried. If the file name is supplied to the program with an extension, for example TEST.XXX or TEST.DDAT, the procedure used is slightly different. In this case, the program will attempt to read the file successively in each format until it is successfully read.

On occasion, it may be necessary to specify the file format to be used. This may be done by following the file name with a /FORMAT= and the file format: filename[.ext]/FORMAT=DUPONT. When the filename is specified on the command line, the /FORMAT= qualifier may be abbreviated, but must be used. However, if the filename is specified in response to a prompt from the program, the string FORMAT= may be omitted: filename.ext/DUPONT.

Dupont. Dupont binary format files contain diffractogram data and optionally peaks and baseline points. The default file extension is `.DDAT`; FORMAT=DUPONT.

NIST (NBS). The NIST format is a simple ASCII format for raw intensity data. The file contains two header lines followed by intensity values as either counts per second or counts, ten per line. The count time is not stored, so ESD's are computed assuming the intensity values are stored as counts. The default file extension is `.NBS`; FORMAT=NIST.

GSAS. The programs can read some of the ASCII GSAS Standard Powder Data files used as input to GSAS (BINTYP='CONST', optionally with ESD's). See the GSAS manual for details. The default file extension is `.GSAS`; FORMAT=GSASASC. In addition, information can also be read from GSAS histogram and reflection files (refinement output). The program must read several files, including the `.EXP`, the `.REFxxP` file and the `.Pxx` file. The default file extension is `.EXP`; FORMAT=GSASHIST.

BNLX7A. This is the format used for data recorded at the Brookhaven NSLS X7A (formerly X13A) instrument. The source flux changes with ring current so intensities are recorded with both scaler and monitor values versus either Q or 2θ. After reading, Intensities are scaled to constant monitor counts. The default file extension is `.X7A`; FORMAT=BNLX7A.

JONES. This highly complex format was developed by Glover Jones of DuPont. It consists of one angle and one intensity value (format `2F10.3`) per line, with no header information. Data need not be recorded with equal steps of 2θ, but the first two lines must have decimal points (.) in columns 7 and 17. The default file extension is `.JONES`; FORMAT=JONES.

IPNS. Binary files produced by the Penn versions of Argonne Intense Pulsed Neutron Source (IPNS) GLASS package and TOF package may be read: the file types that can be read are Radial Distribution Functions, rho(r), g(r), n(r), (default file extension `.RDF`, FORMAT=IPNSRHO, IPNSGOFR, IPNSNOFR); Structure factors, S(Q), S(d) (default file extension `.SOQ`, FORMAT=IPNSSOFQ, IPNSSOFD) ASCII raw counts from .RUN files written by RUNPLT (default file extension `.TOF`, FORMAT=IPNSTOFx where x = T for time, L for wavelength, Q for Q and D for d-spaces) Argonne TOF Rietveld .PLT files written by TOFLS (default file extension `.PLT`, FORMAT=IPNSRIETxy where x = T for time, L for wavelength, Q for Q and D for d-spaces and y = O for the observed, background subracted pattern, C for the computed pattern and D differences [obs-calc]).

PHILIPS – Nova. This format corresponds to an ASCII data file created by the Philips APD system running on a Data General Nova computer. The file contains a single header line with the step size, the starting and the ending angle, followed by intensity values as either counts per second or counts, ten per line. The count time is not stored, so ESD's are computed assuming values in counts. The source radiation is assumed to be both Cu $K\alpha_1$. The default file extension is `.RD`; FORMAT=APDNOVA.

PHILIPS – VAX. This format corresponds to an binary data file created by the Philips 3720 APD system running on a VAX/VMS computer and two associated peak files, one ASCII and one binary. The binary data file consists of fixed length, 512 byte records and the default file extension is `.RD`. The binary format peak file also has 512 byte records and has a default extension of `.DI`. The ASCII peak file is the contents of a peak report from the APD 3720 and has a default extension of `.APLIS`; The FORMAT is APDVAX for all of these files.

SCINTAG – VAX. This format corresponds to an binary data file created by the Scintag system running on a VAX/VMS and two associated peak files. The data file consists of fixed length, 4 byte records and the default file extension is `.RD`. The binary format peak file also has 4 byte records and has default file extension is `.PK`. The ASCII format peak file has default extension `.PKLST`. Since the x-ray tube type is not stored, the radiation is assumed to be both Cu Kα_1 and Kα_2. FORMAT=SCINTAG.

Penn State University "ASCII data file" and "Standard D-I format" peak files. The data file has a title for the first line. The second line contains the starting, ending angles, step size and count time (Format `4F10.0`). The remainder of the file has 10 intensity values (as counts) per line (Format `10F8.0`). The default data file extension is `.ASC`. The peak file has any number of header lines, followed by a card with "`PEAK`" in the first four columns. Remaining lines have one d-space and one peak height per line (Format `14X,F8.4,2X,F3.0`). The default peak file extension is `.ADR`.

In addition to the peak files associated with data files, several additional peak files may be read. They all use FORMAT=PEAK.

SEARCH temporary (peak) files. The temporary files with lists of peak positions may be read by other programs as a peak file. For example, if peaks are entered into SEARCH for use in identification of an unknown pattern, the same peak list may be displayed along with peak positions from JCPDS-ICDD cards in program LOGIC. The default file extension is `.SEA_IN`.

Free Format peak file. The first line in this file is read as a title and the second line (format `F10.0`) is a wavelength. The wavelength should be zero if peak positions have been entered as d-spaces and non-zero for 2θ angles. Remaining lines have one d-space and one peak height per line (Format `2F10.0`). Note that positions and heights may be separated by a comma, if the position and both preceeding and following spaces are less than 10 characters. For example `10.01, 99.` is valid. These files must have extension `.PEAK` to be read.

Chapter 2: Program LOGIC

Program LOGIC is used to search the ICDD-JCPDS database for materials with selected characteristics. The ICDD-JCPDS database contains approximately 60,000 sets of summarized diffraction patterns. The database is copyright by the International Centre for Diffraction Data and may be used only by license. This program maintains a working subset of the full database, referred to as the "current table" where the contents of the table may be increased or decreased according to logical criteria set by the user.

There are five basic categories of instructions that may be given to LOGIC. Commands READ and WRITE are used to read in or write out a stored table; commands TABLES, BROWSE, and INDEX are used to examine the entries in the current table; commands ADD, MATCH and CULL modify the current list by applying logical criteria; command WAVELENGTH controls whether the program will use d-spaces or 2θ angles for input and output; and command `DELETED` controls usage of "deleted" patterns. commands DCL, FILE, HELP and EXIT are used for program control.

The following element symbols are defined within program LOGIC:

> H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr

In addition, the following special symbols are defined for chemical groups or columns in the periodic table:

LN Lanthanides (La - Lu)

AD Actinides (Ac - Lr)

1a period 1 (H,Li,Na,K,Rb,Cs,Fr)

2a period 2 (Be,Mg,Ca,Sr,Ba,Ra)

3a period 3 (B,Al,Ga,In,Tl)

4a period 4 (C,Si,Ge,Sn,Pb)

5a period 5 (N,P,As,Sb,Bi)

6a period 6 (O,S,Se,Te,Po)

7a period 7 (H,F,Cl,Br,I,At)

8a period 8 (He,Ne,Ar,Kr,Xe,Rn)

1b transition metals period 9 (Cu,Ag,Au)

2b transition metals period 10 (Zn,Cd,Hg)

3b transition metals period 1 (Sc,Y,La,Ac)

4b transition metals period 2 (Ti,Zr,Hf)

5b transition metals period 3 (V,Nb,Ta)

6b transition metals period 4 (Cr,Mo,W)

7b transition metals period 5 (Mn,Tc,Re)

8b transition metals period 6-8 (Fe,Co,Ni,Ru,Rh,Pd,Os,Ir,Pt)

2.1 Command ADD (OR)

Command ADD increases the number of entries in the current table using a logical .OR. operation to add all entries which match a specified logical criterion. Command OR is completely equivalent to command ADD.

There are four possible logical criteria that may be established:

- `/ELEMENTS` A list of entries is specified by a partial or complete elemental composition
- `/CARD` A list of entries is specified by ICDD-JCPDS number
- `/PEAKS` A list of entries is specified by positions of the major peaks in the pattern.
- `/COUNT` A list of entries is specified by the number of different elements in the chemical formula.

Qualifiers may be specified in only certain combinations. Square brackets (`[ ]`) indicate parameters that are allowed but are not required. For example, if `/ELEMENTS/OPTIONAL` is used, `/EXACT` is assumed, and need not be specified explicitly. Angle brackets (`< >`) indicate that only one of the enclosed parameters may be chosen. For example, for `/PEAKS/OR` either `/DSPACE` or `/WAVELENGTH` may be used, but not both. Curly brackets (`{ }`) indicate that more than one of the enclosed parameters may be chosen, but at least one must be chosen. For example, either `/OPTIONAL` or `/I_SPAN` or both may be specified with `/ELEMENTS` but one of the two must be specified, unless `/OR` or `/AND` or `/EXACT` is used.

```
ADD {/ELEMENTS= /E_SPAN=} /OR
ADD {/ELEMENTS= /E_SPAN=} /AND
ADD {/ELEMENTS= /E_SPAN=} /EXACT
ADD {/ELEMENTS= /E_SPAN=} {/OPTIONAL= /O_SPAN=} [/EXACT]

ADD/CARDS

ADD/COUNT=

ADD/PEAKS=/OR/FAST  [/ERROR=] [/LEVEL=] </DSPACE /WAVELENGTH=]>
ADD/PEAKS=/AND/FAST [/ERROR=] [/LEVEL=] </DSPACE /WAVELENGTH=]>
ADD/PEAKS=/OR/EXACT/ERROR=  [/LEVEL=] </DSPACE /WAVELENGTH]>
ADD/PEAKS=/AND/EXACT/ERROR= [/LEVEL=] </DSPACE /WAVELENGTH]>
```

The `/ELEMENTS` (or `/E_SPAN`), `/CARD` or `/PEAKS` qualifier should be specified before other all other qualifiers.

QUALIFIERS

`/ELEMENTS=required_list`
`/ELEMENTS`
`/E_SPAN=req_range(s)`

Use this options to specify a list of elements which must be present for the logical criterion to be matched. The list of elements may be used in one of four different ways:

`/OR` An entry with a composition containing any one of the specified elements is a match.

`/AND` An entry with a composition containing all of the specified elements is a match.

`/EXACT` An entry with a composition containing all of the specified elements and no others is a match.

`/OPTIONAL` (and/or `/O_SPAN`) An entry with a composition containing all of the specified elements and any or none of the optional elements, but no others no others is a match.

Use `/E_SPAN` to specify a range of elements which must be present for the logical criterion to be matched. This option is equivalent to specifying the elements individually in the `required_list` using `/ELEMENTS`.

Examples of the use of these qualifiers are:

`/ELEMENTS=SI`

`/elem=(si,o,H)`

`/E_SPAN=(H,BE)`

`/E_SPAN=(Be,H)` (same as previous)

`/ELEMENTS=(H,HE,LI,BE)` (same as previous)

`/E_SPAN=(H,BE,C,F)` (specifies two ranges: from H to Be and from C to F.

Note that capitalization is ignored and the elements must be surrounded by parentheses and separated by commas, if more than one element is specified. For the `/E_SPAN` qualifier, element ranges may be specified in either ascending or descending order. To specify more than one range, specify more than one pair of endpoints. If no elements are specified with `/ELEMENTS`, and `/E_SPAN` is not used, the program will prompt for elements.

The following qualifiers may not be used with `/ELEMENTS` or `/E_SPAN`: `/CARDS`, `/PEAKS`, `/FAST`, `/ERROR`, or `/LEVEL`. The `/ELEMENTS` or `/E_SPAN` qualifier should be specified before other all other qualifiers.

`/COUNT=elm_count`
`/COUNT=(c_min,c_max)`
`/COUNT`

Use this qualifier to select entries using the number of unique elements in the chemical formula. The qualifier may be used three ways, if a single value is specified, for example `/COUNT=2`, then entries are selected with that single number of elements. If two values are used, for example `/COUNT=(2,4)` the two numbers represent a range of values, in this case 2, 3 or 4 elements are allowed. If no value is specified, the computer will prompt for one or more values.

Note that Cr2O3 . xH2O will be counted as having 3 elements in the formula.

No other qualifiers are allowed with `/COUNT`.

`/CARDS=card_list`
`/CARDS`

Use this qualifier to select entries using their ICDD-JCPDS entry number. The entry number is always a five or six digit number consisting of the "old" entry number plus 10,000 times the set number. For example, entry 413 in set 7 would be coded as:

> `/CARD=70413` or
>
> `/CARD=070413`

To specify more than one entry, separate the list with commas and enclose the list in parentheses:

> `/CARD=(070413,10001)`

No other qualifiers are allowed with use of the `/CARDS` qualifier.

`/PEAKS=peak_list`
`/PEAKS`

Use this option to select entries based on the location of the intense peaks in the pattern. The peak positions must be input as either 2θ angles or as d-spaces depending on the current wavelength setting (see command WAVELENGTH). The wavelength setting may be overridden using the `/WAVELENGTH` or the `/DSPACE` qualifiers.

All entries with intense peaks (the intensity threshold is set by the `/LEVEL` option) within some region around input peak position will be selected. The actual window depends on the value(s) used on the `/ERROR` option. If more than one peak is input, the peaks should be separated by commas and enclosed in parentheses. The list of peaks may be used in one of two different ways:

> `/OR` An entry with a composition containing any one of the specified peaks is a match.
>
> `/AND` An entry with a composition containing all of the specified peaks is a match.

If no peaks are input, the program will prompt for a list of peaks.

The following qualifiers may not be used with `/PEAKS`: `/CARDS`, `/ELEMENTS`, `/E_SPAN`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`. Specify `/PEAKS` as the first qualifier on the line.

`/ERROR=error_list`

The `error_list` specifies an allowed range for each peak. The range is used in one of two ways, depending on mode used by the program. If the mode is `/EXACT`, the error range is used exactly as specified. For example, If `/PEAK=15.5/ERROR=0.1/EXACT` is used, peaks at locations between 15.4 and 15.6 will be selected. The other mode, `/FAST`, may be considerably more rapid than `/EXACT`. In `/FAST` mode, the range specified with `/ERROR` is expanded to match spacing of records in the peak index files. For example, if the peak index records cover the ranges, 15.15-15.3, 15.3-15.45, 15.45-15.6, etc., then if `/PEAK=15.5/ERROR=0.1/FAST` is used, then the error range will be expanded to select peaks between 15.3 and 15.6.

An error value may be specified for each peak, but if the number of values in the `error_list` is less than the number of peaks in the `peak_list`, the last error value will be used for all remaining peaks. If the `/ERROR` parameter is not used, the program will prompt for a single error value for all peaks. The error value should be specified in the same units (d-space or 2θ) as the peak positions.

The `/PEAKS` qualifier must precede this qualifier. The following qualifiers may not be used with `/ERROR`: `/CARDS`, `/ELEMENTS`, `/E_SPAN`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`.

`/DSPACE` Using this qualifier overrides the current wavelength setting and forces peaks to be input as d-spaces. This qualifier cannot be used with `/WAVELENGTH` and will be ignored if used with a qualifier other than `/PEAKS`.

`/WAVELENGTH=wave_length` Using this qualifier overrides the current wavelength setting and forces peaks to be input as 2θ angles at `wave_length`Å. This qualifier cannot be used with `/DSPACE` and will be ignored if used with a qualifier other than `/PEAKS`.

`/LEVEL=peak_level` Specifies a relative intensity threshold for peak positions specified with the `/PEAKS` qualifier. The threshold value is used slightly differently in `/FAST` mode versus `/EXACT` mode. In `/EXACT` mode, the value specifies the exact intensity threshold (in percent relative intensity). For example if `/PEAKS=20.5/ERR=0.1/LEVEL=75/DSPACE/EXACT` is specified, entries with peaks having d-spaces from 20.4 to 20.6 Å with relative intensities of 75% or greater will be located. In `/FAST` mode, the threshold value specifies a peak index to be searched. If there is no peak index at this value, a peak index with a lower threshold is used (at 10 % increments). Thus in the example `/PEAKS=20.5/ERR=0.1/LEVEL=75/DSPACE/FAST`, the error range is opened (see `/ERROR`) and the intensity threshold is also possibly lowered, so that potentially more entries will be selected than in `/EXACT` mode. It is also possible to specify `/LEVEL=3s` in `/FAST` mode. This specifies an index of the three strongest peaks in each entry.

The `/PEAKS` qualifier must precede this qualifier. The following qualifiers may not be used with `/LEVEL`: `/CARDS`, `/ELEMENTS`, `/E_SPAN`, `/COUNT` `/OPTIONAL`, or `/O_SPAN`.

`/EXACT` Use `/EXACT` with `/ELEMENTS` to specify that only entries containing all of the specified elements and no others match as the specified logical criterion. It is possible to widen this criterion so that certain elements are allowed, but not required, using the `/OPTIONAL` and/or `/O_SPAN` qualifiers.

Use `/EXACT` with `/PEAKS` to specify that the error range specified for peak positions should not be extended, but instead be used as given. (See the description given for `/ERROR`.)

The following qualifiers may not be used with `/EXACT` and `/ELEMENTS`: `/CARDS`, `/PEAKS`, `/OR`, `/AND`, `/ERROR`, `/FAST`, `/COUNT` or `/LEVEL`.

The following qualifiers may not be used with /EXACT and /PEAKS: /CARDS, /ELEMENTS, /E_SPAN, /FAST, /COUNT /OPTIONAL, or /O_SPAN.

/FAST

Use /FAST with /PEAKS to specify that the error range specified for peak positions may be extended for most efficient searching. (See the description given for /ERROR.)

The following qualifiers may not be used with /FAST: /CARDS, /ELEMENTS, /E_SPAN, /OPTIONAL, /EXACT, /COUNT or /O_SPAN.

/OR

Use /OR with either /PEAKS or /ELEMENTS to specify that any entry containing the specified element or peak is a match for the specified logical criterion.

The following qualifiers may not be used with /OR: /CARDS, /AND, /COUNT, /OPTIONAL, or /O_SPAN. Also, if /ELEMENTS and /OR are used, /EXACT cannot be used.

/AND

Use /AND with either /PEAKS or /ELEMENTS to specify that only entries containing all of the specified elements or peaks match for the specified logical criterion.

The following qualifiers may not be used with /AND: /CARDS, /OR, /COUNT, /OPTIONAL, or /O_SPAN. Also, if /ELEMENTS and /AND are used, /EXACT cannot be used.

/OPTIONAL=optional_list
/O_SPAN=opt_range(s)

Use /OPTIONAL or /O_SPAN with /ELEMENTS to specify that only entries containing all of the required elements specified in the required_list (see /ELEMENTS and /E_SPAN) and optionally those in the optional_list, but no others, as the specified logical criterion. /O_SPAN is equivalent to /OPTIONAL except that ranges of elements may be specified.

Examples of the use of this qualifier are:

/OPTIONAL=SI

/ig=(si,o,H)

/O_SPAN=(H,BE)

/O_SPAN=(BE,H) (equivalent to previous)

/OPTIONAL=(H,HE,LI,BE) (equivalent to previous)

/O_SPAN=(H,BE,C,F) specifies two ranges: from H to Be and from C to F.

Note that capitalization is ignored and the elements must be surrounded by parentheses and separated by commas, if more than one element is specified. Ranges may be specified in either ascending or descending order. To specify more than one range, specify more than one pair of endpoints.

The following qualifiers may not be used with /OPTIONAL or /O_SPAN: /CARDS, /PEAKS, /FAST, /OR, /AND, /ERROR, /COUNT, or /LEVEL. Qualifier /EXACT is assumed to be present if /OPTIONAL or /O_SPAN is used and thus is optional. /O_SPAN may be used with /OPTIONAL.

2.2 Command BROWSE

Use this function to examine tables of angles or d-spaces for all entries in the "current list" from a terminal. Entries are displayed one at a time; it is possible to page backwards or forwards in the list and to print selected entries. If the full ICDD-JCPDS (PDF-2) database is on-line, the entire ICDD-JCPDS entry may be displayed or printed.

After entering the BROWSE command, a prompt line is displayed, which shows the total number of entries in the current list and the relative position of the current entry within the list. Also displayed is a list of available commands. The following commands are defined:

`+n_p` moves forward in the list by `n_p` entries;

`-n_p` moves backward by `n_p` entries;

`>n_p` displays the `n_p`-th entry in the list;

`[crd` displays ICDD-JCPDS entry `crd`, or the closest entry in the list by number;

(blank line) displays the next entry;

`P` prints the chemical information and D/I data (PDF-1 data) for the current entry and advances to the next entry;

`C` culls (removes) the current entry from the current table and advances to the next entry;

`D` displays all the information for the current entry in the full ICDD-JCPDS (PDF-2) database;

`A` prints All the information for the current entry and advances to the next entry;

`G` graphically displays one or more entries, starting from the current entry;

`^Z` or advancing past the last entry terminates BROWSE mode.

The command letter or symbol, (`+`, `>` or `P`, for example) must be the first letter on the line. Commands which are not valid are not given in the list of options. Commands D and A both require the PDF-2 database either on disk or on CD-ROM. If the PDF-2 database is unavailable, these options will not be listed. The graph command, G, is only available on graphics-compatible terminals. This command can be used to display experimental data as well as ICDD-JCPDS entries. Each time the command is called, one can input a data or peak file to the program and this data will be displayed as well as the selected entries. A wide variety of peak and data files may be read see the section on File_formats in the first chapter. Of particular use will be SEARCH temporary files, which may be read directly at this point by LOGIC and may then then be plotted.

2.3 Command COMMENT

The program records a summary of the logical steps (commands that modify the contents of the current table). Use this command to place a comment line into the list of logical steps. The comment may be placed on the same line as the COMMENT command, or will be prompted.

PARAMETER

`comment_line` A single line of comments may be placed after the COMMENT command. Lowercase letters will be translated to uppercase if the `comment_line` is placed on the same line, rather than entered at the prompt.

2.4 Command CULL (NAND)

Command CULL decreases the number of entries in the current table using a logical .AND. .NOT. operation to remove all entries which match a specified logical criterion. Command NAND is completely equivalent to command CULL.

There are five possible logical criteria that may be established:

- `/ELEMENTS` A list of entries is specified by a partial or complete elemental composition
- `/CARD` A list of entries is specified by number
- `/PEAKS` A list of entries is specified by positions of the major peaks in the pattern.
- `/NAME` A list of entries is specified by chemical/mineral name
- `/COUNT` A list of entries is specified by the number of different elements in the chemical formula.

Qualifiers may be specified in only certain combinations. Square brackets (`[ ]`) indicate parameters that are allowed but are not required. For example, if `/ELEMENTS/OPTIONAL` is used, `/EXACT` is assumed, and need not be specified explicitly. Angle brackets (`< >`) indicate that only one of the enclosed parameters may be chosen. For example, for `/PEAKS/OR` either `/DSPACE` or `/WAVELENGTH` may be used, but not both. Curly brackets (`{ }`) indicate that more than one of the enclosed parameters may be chosen, but at least one must be chosen. For example, either `/OPTIONAL` or `/I_SPAN` or both may be specified with `/NOELEMENTS` but one of the two should be specified.

```
CULL {/ELEMENTS= /E_SPAN=} /OR
CULL {/ELEMENTS= /E_SPAN=} /AND
CULL {/ELEMENTS= /E_SPAN=} /EXACT
CULL {/ELEMENTS= /E_SPAN=} {/OPTIONAL= /O_SPAN=} [/EXACT]
CULL/NOELEMENTS {/OPTIONAL= /O_SPAN=} [/EXACT]

CULL/CARDS=

CULL/NAME=

CULL/COUNT=

CULL/PEAKS=/OR/FAST  [/ERROR=] [/LEVEL=] </DSPACE /WAVELENGTH=]>
CULL/PEAKS=/AND/FAST [/ERROR=] [/LEVEL=] </DSPACE /WAVELENGTH=]>
CULL/PEAKS=/OR/EXACT/ERROR=  [/LEVEL=] </DSPACE /WAVELENGTH=]>
CULL/PEAKS=/AND/EXACT/ERROR= [/LEVEL=] </DSPACE /WAVELENGTH=]>
```

The `/ELEMENTS` (or `/E_SPAN`), `/CARD`, `/NAME` or `/PEAKS` qualifier should be specified before other all other qualifiers.

QUALIFIERS

`/ELEMENTS=required_list`
`/ELEMENTS`
`/NOELEMENTS`
`/E_SPAN=req_range(s)`

Use this options to specify a list of elements which must be present for the logical criterion to be matched. The list of elements may be used in one of four different ways:

- `/OR` An entry with a composition containing any one of the specified elements is a match.
- `/AND` An entry with a composition containing all of the specified elements is a match.
- `/EXACT` An entry with a composition containing all of the specified elements and no others is a match.
- `/OPTIONAL` (and/or `/O_SPAN`) An entry with a composition containing all of the specified elements and any or none of the optional elements, but no others no others is a match.

Use `/E_SPAN` to specify a range of elements which must be present for the logical criterion to be matched. This option is equivalent to specifying the elements individually in the `required_list` using `/ELEMENTS`.

The `/NOELEMENTS` option is used if there are no required elements, but optional elements will be specified using the `/OPTIONAL` or `/O_SPAN` options. Thus, entries will be removed that have any combination of the optional elements and no others. Use of this option will remove all entries with unassigned chemical formulas, as would be performed by a `CULL/COUNT=0` command.

Examples of the use of these qualifiers are:

`/ELEMENTS=SI`

`/elem=(si,o,H)`

`/E_SPAN=(H,BE)`

`/E_SPAN=(Be,H)` (same as previous)

`/ELEMENTS=(H,HE,LI,BE)` (same as previous)

`/E_SPAN=(H,BE,C,F)` (specifies two ranges: from H to Be and from C to F.

Note that capitalization is ignored and the elements must be surrounded by parentheses and separated by commas, if more than one element is specified. For the `/E_SPAN` qualifier, element ranges may be specified in either ascending or descending order. To specify more than one range, specify more than one pair of endpoints. If no elements are specified with `/ELEMENTS`, and `/E_SPAN` is not used, the program will prompt for elements.

The following qualifiers may not be used with `/ELEMENTS` or `/E_SPAN`: `/CARDS`, `/NAME`, `/PEAKS`, `/FAST`, `/ERROR`, or `/LEVEL`. The `/ELEMENTS` or `/E_SPAN` qualifier should be specified before other all other qualifiers.

`/COUNT=elm_count`
`/COUNT=(c_min,c_max)`
`/COUNT`

Use this qualifier to select entries using the number of unique elements in the chemical formula. The qualifier may be used three ways, if a single value is specified, for example `/COUNT=2`, then entries are selected with that single number of elements. If two values are used, for example `/COUNT=(2,4)` the two numbers represent a range of values, in this case 2, 3 or 4 elements are allowed. If no value is specified, the computer will prompt for one or more values.

Note that Cr2O3 . xH2O will be counted as having 3 elements in the formula.

No other qualifiers are allowed with `/COUNT`.

`/CARDS=card_list`
`/CARDS`

Use this qualifier to select entries using their ICDD-JCPDS entry number. The entry number is always a five or six digit number consisting of the "old" entry number plus 10,000 times the set number. For example, entry 413 in set 7 would be coded as:

`/CARD=70413` or

`/CARD=070413`

To specify more than one entry, separate the list with commas and enclose the list in parentheses:

`/CARD=(070413,10001)`

No other qualifiers are allowed with use of the `/CARDS` qualifier.

`/NAME=compound_name`
`/NAME=mineral_name`

A fragment of a chemical or mineral name to be matched. The name listed on an entry must match the `compound_name` fragment letter for letter (lowercase letters will be converted to uppercase). If spaces are to be included in the fragment, the fragment should be enclosed in quotation marks ("). For example,

`/NAME=silicon`

`/NAME="silicon oxide"`

No other qualifiers may be used with `/NAME`.

`/PEAKS=peak_list`
`/PEAKS`

Use this option to select entries based on the location of the intense peaks in the pattern. The peak positions must be input as either 2θ angles or as d-spaces depending on the current wavelength setting (see command WAVELENGTH). The wavelength setting may be overridden using the `/WAVELENGTH` or the `/DSPACE` qualifiers.

All entries with intense peaks (the intensity threshold is set by the `/LEVEL` option) within some region around input peak position will be selected. The actual window depends on the value(s) used on the `/ERROR` option. If more than one peak is input, the peaks should be separated by commas and enclosed in parentheses. The list of peaks may be used in one of two different ways:

`/OR` An entry with a composition containing any one of the specified peaks is a match.

`/AND` An entry with a composition containing all of the specified peaks is a match.

If no peaks are input, the program will prompt for a list of peaks.

The following qualifiers may not be used with `/PEAKS`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`. Specify `/PEAKS` as the first qualifier on the line.

`/ERROR=error_list` — The `error_list` specifies an allowed range for each peak. The range is used in one of two ways, depending on mode used by the program. If the mode is `/EXACT`, the error range is used exactly as specified. For example, If `/PEAK=15.5/ERROR=0.1/EXACT` is used, peaks at locations between 15.4 and 15.6 will be selected. The other mode, `/FAST`, may be considerably more rapid than `/EXACT`. In `/FAST` mode, the range specified with `/ERROR` is expanded to match spacing of records in the peak index files. For example, if the peak index records cover the ranges, 15.15-15.3, 15.3-15.45, 15.45-15.6, etc., then if `/PEAK=15.5/ERROR=0.1/FAST` is used, then the error range will be expanded to select peaks between 15.3 and 15.6.

An error value may be specified for each peak, but if the number of values in the `error_list` is less than the number of peaks in the `peak_list`, the last error value will be used for all remaining peaks. If the `/ERROR` parameter is not used, the program will prompt for a single error value for all peaks. The error value should be specified in the same units (d-space or 2θ) as the peak positions.

The `/PEAKS` qualifier must precede this qualifier. The following qualifiers may not be used with `/ERROR`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`.

`/DSPACE` — Using this qualifier overrides the current wavelength setting and forces peaks to be input as d-spaces. This qualifier cannot be used with `/WAVELENGTH` and will be ignored if used with a qualifier other than `/PEAKS`.

`/WAVELENGTH=wave_length` — Using this qualifier overrides the current wavelength setting and forces peaks to be input as 2θ angles at `wave_length`Å. This qualifier cannot be used with `/DSPACE` and will be ignored if used with a qualifier other than `/PEAKS`.

`/LEVEL=peak_level` — Specifies a relative intensity threshold for peak positions specified with the `/PEAKS` qualifier. The threshold value is used slightly differently in `/FAST` mode versus `/EXACT` mode. In `/EXACT` mode, the value specifies the exact intensity threshold (in percent relative intensity). For example if `/PEAKS=20.5/ERR=0.1/LEVEL=75/DSPACE/EXACT` is specified, entries with peaks having d-spaces from 20.4 to 20.6 Å with relative intensities of 75% or greater will be located. In `/FAST` mode, the threshold value specifies a peak index to be searched. If there is no peak index at this value, a peak index with a lower threshold is used (at 10 % increments). Thus in the example `/PEAKS=20.5/ERR=0.1/LEVEL=75/DSPACE/FAST`, the error range is opened (see `/ERROR`) and the intensity threshold is also possibly lowered, so that potentially more entries will be selected than in `/EXACT` mode. It is also possible to specify `/LEVEL=3s` in `/FAST` mode. This specifies an index of the three strongest peaks in each entry.

The /PEAKS qualifier must precede this qualifier. The following qualifiers may not be used with /LEVEL: /CARDS, /NAME, /ELEMENTS, /E_SPAN, /COUNT /OPTIONAL, or /O_SPAN.

/EXACT

Use /EXACT with /ELEMENTS to specify that only entries containing all of the specified elements and no others match as the specified logical criterion. It is possible to widen this criterion so that certain elements are allowed, but not required, using the /OPTIONAL and/or /O_SPAN qualifiers.

Use /EXACT with /PEAKS to specify that the error range specified for peak positions should not be extended, but instead be used as given. (See the description given for /ERROR.)

The following qualifiers may not be used with /EXACT and /ELEMENTS: /CARDS, /NAME, /PEAKS, /OR, /AND, /ERROR, /FAST, /COUNT or /LEVEL.

The following qualifiers may not be used with /EXACT and /PEAKS: /CARDS, /NAME, /ELEMENTS, /E_SPAN, /FAST, /COUNT /OPTIONAL, or /O_SPAN.

/FAST

Use /FAST with /PEAKS to specify that the error range specified for peak positions may be extended for most efficient searching. (See the description given for /ERROR.)

The following qualifiers may not be used with /FAST: /CARDS, /NAME, /ELEMENTS, /E_SPAN, /OPTIONAL, /EXACT, /COUNT or /O_SPAN.

/OR

Use /OR with either /PEAKS or /ELEMENTS to specify that any entry containing the specified element or peak is a match for the specified logical criterion.

The following qualifiers may not be used with /OR: /CARDS, /NAME, /AND, /COUNT, /OPTIONAL, or /O_SPAN. Also, if /ELEMENTS and /OR are used, /EXACT cannot be used.

/AND

Use /AND with either /PEAKS or /ELEMENTS to specify that only entries containing all of the specified elements or peaks match for the specified logical criterion.

The following qualifiers may not be used with /AND: /CARDS, /NAME, /OR, /COUNT, /OPTIONAL, or /O_SPAN. Also, if /ELEMENTS and /AND are used, /EXACT cannot be used.

/OPTIONAL=optional_list
/O_SPAN=opt_range(s)

Use /OPTIONAL or /O_SPAN with /ELEMENTS to specify that only entries containing all of the required elements specified in the required_list (see /ELEMENTS and /E_SPAN) and optionally those in the optional_list, but no others, as the specified logical criterion. /O_SPAN is equivalent to /OPTIONAL except that ranges of elements may be specified.

Examples of the use of this qualifier are:

```
/OPTIONAL=SI
/ig=(si,o,H)
/O_SPAN=(H,BE)
```

`/O_SPAN=(BE,H)` (equivalent to previous)

`/OPTIONAL=(H,HE,LI,BE)` (equivalent to previous)

`/O_SPAN=(H,BE,C,F)` specifies two ranges: from H to Be and from C to F.

Note that capitalization is ignored and the elements must be surrounded by parentheses and separated by commas, if more than one element is specified. Ranges may be specified in either ascending or descending order. To specify more than one range, specify more than one pair of endpoints.

The following qualifiers may not be used with `/OPTIONAL` or `/O_SPAN`: `/CARDS`, `/NAME`, `/PEAKS`, `/FAST`, `/OR`, `/AND`, `/ERROR`, `/COUNT`, or `/LEVEL`. Qualifier `/EXACT` is assumed to be present if `/OPTIONAL` or `/O_SPAN` is used and thus is optional. `/O_SPAN` may be used with `/OPTIONAL`.

2.5 Command DCL

Spawns a subprocess to execute DCL commands, type LOGOUT to return back to LOGIC without affecting the "current list". This command is useful for quick DCL "errands" such as answering a mail message without exiting the program.

2.6 Command DELETED

Some of the entries in the database are marked as "deleted" by the editors of the database. If these entries are included in the database (using the ENCODE program, PDF1) it is possible to select that these entries will be included or excluded from the operations of this program.

This command causes logical name `PS_DELETED` to be set so that subsequent operations with the program and with other programs in the Powder Suite package will use the same option. The default mode for the program is `DELETED/EXCLUDE`. However, if desired the `PS_DELETED` logical name may be predefined (see customization instructions) to change the default.

QUALIFIERS

`/INCLUDE` Specifies that deleted entries will be included in the logical operations.

`/EXCLUDE` Specifies that deleted entries will be not be included in the logical operations.

2.7 Command EXIT

Type EXIT (which can be abbreviated to EX) to exit from the program. Alternately, press Control Z (`^Z`) to exit.

2.8 Command FILE

Allows a series of commands to be input to the program from an external file. The file should be prepared before starting the program, or using the DCL command to invoke an editor.

PARAMETER

`file_name` A single file may be specified on the command line containing the name of the file with commands. If the file is not specified, a prompt will be given to request a file name.

If no file extension is supplied, the default extension is `.CMD`

2.9 Command HELP

Invokes the VAX/VMS online help facility for help on this program.

2.10 Command INDEX

Displays an index of the entries in the current list, with the information for each entry summarized to a single line.

There are three possible formats: In "names" format, the chemical composition, chemical and mineral name for each entry in the current list are given. In "Hanawalt" format, the most intense lines are listed with intensity and d-spacing or angle. This list may optionally be sorted in order of increasing d-space or angle and the most intense lines may be permuted. In "maxD" format, the lines are listed in order of decreasing d-space (or increasing angle). This list may be sorted and permuted, as before.

If `/PRINT` is not specified, the list is displayed on the terminal in sections. After each section, a "`Continue?`" prompt appears. If the response is "`N`", "`P`" or `^Z`, no more sections will be displayed. If "`P`" is specified, the complete list will be printed. Enter "`Y`" or a blank line for the next section.

QUALIFIERS

`/HANAWALT=sort_lines`
`/HANAWALT`

The list is displayed in Hanawalt format – an entry number followed by the d-spaces or angles ordered by intensity.

Entries are listed by PDF file in sequential order, unless the `sort_lines` option is specified, in which case the records are sorted by increasing d-spacing or angle.

`sort_lines` specifies the number of peaks to be used for sorting:

`/HANAWALT=0` – the list is sorted by set and entry number.

`/HANAWALT=1` – the list is sorted based on the most intense line.

`/HANAWALT=sort_lines` – (`sort_lines`=2,3,4 or 5), the `sort_lines` most intense lines are permuted and then sorted, thus the length of the list increases by a factor of `sort_lines`.

`/MAXD=sort_lines`
`/MAXD`

The list is displayed in maxD format – an entry number followed by the d-spaces or angles ordered by decreasing d-space (increasing angle).

Entries are listed by PDF file in sequential order, unless the `sort_lines` option is specified, in which case the records are sorted by increasing d-spacing or angle.

`sort_lines` specifies the number of peaks to be used for sorting:

> `/MAXD=0` – the list is sorted by set and entry number.
>
> `/MAXD=1` – the list is sorted based on the highest d-space line.
>
> `/MAXD=sort_lines` – (`sort_lines`=2,3,4 or 5), the `sort_lines` highest d-space lines are permuted and then sorted, thus the length of the list increases by a factor of `sort_lines`.

`/NAMES`

The "current list" is displayed with chemical formula, compound name and mineral name. Entries are listed in sequential order by set and entry number.

`/PRINT`

Prints the index rather than displaying it on the terminal.

2.11 Command MATCH (AND)

Command MATCH decreases the number of entries in the current table using a logical .AND. operation to remove all entries which do not match a specified logical criterion. Command AND is completely equivalent to command MATCH.

There are five possible logical criteria that may be established:

- `/ELEMENTS` A list of entries is specified by a partial or complete elemental composition
- `/CARD` A list of entries is specified by number
- `/PEAKS` A list of entries is specified by positions of the major peaks in the pattern.
- `/NAME` A list of entries is specified by chemical/mineral name
- `/COUNT` A list of entries is specified by the number of different elements in the chemical formula.

Qualifiers may be specified in only certain combinations. Square brackets (`[ ]`) indicate parameters that are allowed but are not required. For example, if `/ELEMENTS/OPTIONAL` is used, `/EXACT` is assumed, and need not be specified explicitly. Angle brackets (`< >`) indicate that only one of the enclosed parameters may be chosen. For example, for `/PEAKS/OR` either `/DSPACE` or `/WAVELENGTH` may be used, but not both. Curly brackets (`{ }`) indicate that more than one of the enclosed parameters may be chosen, but at least one must be chosen. For example, either `/ELEMENTS` or `/E_SPAN` or both may be specified, but one of the two should be specified.

```
MATCH {/ELEMENTS= /E_SPAN=} /OR
MATCH {/ELEMENTS= /E_SPAN=} /AND
MATCH {/ELEMENTS= /E_SPAN=} /EXACT
MATCH {/ELEMENTS= /E_SPAN=} {/OPTIONAL= /O_SPAN=} [/EXACT]
MATCH/NOELEMENTS {/OPTIONAL= /O_SPAN=} [/EXACT]

MATCH/CARDS=
```

```
MATCH/NAME=

MATCH/COUNT=

MATCH/PEAKS=/OR/FAST  [/ERROR=] [/LEVEL=] </DSPACE /WAVELENGTH=]>
MATCH/PEAKS=/AND/FAST [/ERROR=] [/LEVEL=] </DSPACE /WAVELENGTH=]>
MATCH/PEAKS=/OR/EXACT/ERROR=  [/LEVEL=] </DSPACE /WAVELENGTH=]>
MATCH/PEAKS=/AND/EXACT/ERROR= [/LEVEL=] </DSPACE /WAVELENGTH=]>
```

The `/ELEMENTS` (or `/E_SPAN`), `/CARD`, `/NAME` or `/PEAKS` qualifier should be specified before other all other qualifiers.

QUALIFIERS

`/ELEMENTS=required_list`
`/ELEMENTS`
`/NOELEMENTS`
`/E_SPAN=req_range(s)`

Use this options to specify a list of elements which must be present for the logical criterion to be matched. The list of elements may be used in one of four different ways:

- `/OR` An entry with a composition containing any one of the specified elements is a match.
- `/AND` An entry with a composition containing all of the specified elements is a match.
- `/EXACT` An entry with a composition containing all of the specified elements and no others is a match.
- `/OPTIONAL` (and/or `/O_SPAN`) An entry with a composition containing all of the specified elements and any or none of the optional elements, but no others no others is a match.

Use `/E_SPAN` to specify a range of elements which must be present for the logical criterion to be matched. This option is equivalent to specifying the elements individually in the `required_list` using `/ELEMENTS`.

The `/NOELEMENTS` option is used if there are no required elements, but optional elements will be specified using the `/OPTIONAL` or `/O_SPAN` options. Thus, entries will be selected that have any combination of the optional elements and no others. Use of this option will allow some unexpected entries, entries with unassigned chemical formulas. These entries may be removed using a `CULL/COUNT=0` command.

Examples of the use of these qualifiers are:

`/ELEMENTS=SI`

`/elem=(si,o,H)`

`/E_SPAN=(H,BE)`

`/E_SPAN=(Be,H)` (same as previous)

`/ELEMENTS=(H,HE,LI,BE)` (same as previous)

`/E_SPAN=(H,BE,C,F)` (specifies two ranges: from H to Be and from C to F.

Note that capitalization is ignored and the elements must be surrounded by parentheses and separated by commas, if more than one element is specified. For the `/E_SPAN` qualifier, element ranges may be specified in either ascending or descending order. To specify more than one range, specify more than one pair of endpoints. If no elements are specified with `/ELEMENTS`, and `/E_SPAN` is not used, the program will prompt for elements.

The following qualifiers may not be used with `/ELEMENTS` or `/E_SPAN`: `/CARDS`, `/PEAKS`, `/ERROR`, or `/LEVEL`. The `/ELEMENTS` or `/E_SPAN` qualifier should be specified before other all other qualifiers.

`/COUNT=elm_count`
`/COUNT=(c_min,c_max)`
`/COUNT`

Use this qualifier to select entries using the number of unique elements in the chemical formula. The qualifier may be used three ways, if a single value is specified, for example `/COUNT=2`, then entries are selected with that single number of elements. If two values are used, for example `/COUNT=(2,4)` the two numbers represent a range of values, in this case 2, 3 or 4 elements are allowed. If no value is specified, the computer will prompt for one or more values.

Note that Cr2O3 . xH2O will be counted as having 3 elements in the formula.

No other qualifiers are allowed with `/COUNT`.

`/CARDS=card_list`
`/CARDS`

Use this qualifier to select entries using their ICDD-JCPDS entry number. The entry number is always a five or six digit number consisting of the "old" entry number plus 10,000 times the set number. For example, entry 413 in set 7 would be coded as:

`/CARD=70413` or

`/CARD=070413`

To specify more than one entry, separate the list with commas and enclose the list in parentheses:

`/CARD=(070413,10001)`

No other qualifiers are allowed with use of the `/CARDS` qualifier.

`/NAME=compound_name`
`/NAME=mineral_name`

A fragment of a chemical or mineral name to be matched. The name listed on an entry must match the `compound_name` fragment letter for letter (lowercase letters will be converted to uppercase). If spaces are to be included in the fragment, the fragment should be enclosed in quotation marks ("). For example,

`/NAME=silicon`

`/NAME="silicon oxide"`

No other qualifiers may be used with `/NAME`.

`/PEAKS=peak_list`
`/PEAKS`

Use this option to select entries based on the location of the intense peaks in the pattern. The peak positions must be input as either 2θ angles or as d-spaces depending on the current wavelength setting (see command WAVELENGTH). The wavelength setting may be overridden using the `/WAVELENGTH` or the `/DSPACE` qualifiers.

All entries with intense peaks (the intensity threshold is set by the `/LEVEL` option) within some region around input peak position will be selected. The actual window depends on the value(s) used on the `/ERROR` option. If more than one peak is input, the peaks should be separated by commas and enclosed in parentheses. The list of peaks may be used in one of two different ways:

- `/OR` An entry with a composition containing any one of the specified peaks is a match.
- `/AND` An entry with a composition containing all of the specified peaks is a match.

If no peaks are input, the program will prompt for a list of peaks.

The following qualifiers may not be used with `/PEAKS`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`. Specify `/PEAKS` as the first qualifier on the line.

`/ERROR=error_list`

The `error_list` specifies an allowed range for each peak. The range is used in one of two ways, depending on mode used by the program. If the mode is `/EXACT`, the error range is used exactly as specified. For example, If `/PEAK=15.5/ERROR=0.1/EXACT` is used, peaks at locations between 15.4 and 15.6 will be selected. The other mode, `/FAST`, may be considerably more rapid than `/EXACT`. In `/FAST` mode, the range specified with `/ERROR` is expanded to match spacing of records in the peak index files. For example, if the peak index records cover the ranges, 15.15-15.3, 15.3-15.45, 15.45-15.6, etc., then if `/PEAK=15.5/ERROR=0.1/FAST` is used, then the error range will be expanded to select peaks between 15.3 and 15.6.

An error value may be specified for each peak, but if the number of values in the `error_list` is less than the number of peaks in the `peak_list`, the last error value will be used for all remaining peaks. If the `/ERROR` parameter is not used, the program will prompt for a single error value for all peaks. The error value should be specified in the same units (d-space or 2θ) as the peak positions.

The `/PEAKS` qualifier must precede this qualifier. The following qualifiers may not be used with `/ERROR`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`.

`/DSPACE`

Using this qualifier overrides the current wavelength setting and forces peaks to be input as d-spaces. This qualifier cannot be used with `/WAVELENGTH` and will be ignored if used with a qualifier other than `/PEAKS`.

`/WAVELENGTH=wave_length` Using this qualifier overrides the current wavelength setting and forces peaks to be input as 2θ angles at `wave_length`Å. This qualifier cannot be used with `/DSPACE` and will be ignored if used with a qualifier other than `/PEAKS`.

`/LEVEL=peak_level` Specifies a relative intensity threshold for peak positions specified with the `/PEAKS` qualifier. The threshold value is used slightly differently in `/FAST` mode versus `/EXACT` mode. In `/EXACT` mode, the value specifies the exact intensity threshold (in percent relative intensity). For example if `/PEAKS=20.5/ERR=0.1/LEVEL=75/DSPACE/EXACT` is specified, entries with peaks having d-spaces from 20.4 to 20.6 Å with relative intensities of 75% or greater will be located. In `/FAST` mode, the threshold value specifies a peak index to be searched. If there is no peak index at this value, a peak index with a lower threshold is used (at 10 % increments). Thus in the example `/PEAKS=20.5/ERR=0.1/LEVEL=75/DSPACE/FAST`, the error range is opened (see `/ERROR`) and the intensity threshold is also possibly lowered, so that potentially more entries will be selected than in `/EXACT` mode. It is also possible to specify `/LEVEL=3s` in `/FAST` mode. This specifies an index of the three strongest peaks in each entry.

The `/PEAKS` qualifier must precede this qualifier. The following qualifiers may not be used with `/LEVEL`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/COUNT` `/OPTIONAL`, or `/O_SPAN`.

`/EXACT` Use `/EXACT` with `/ELEMENTS` to specify that only entries containing all of the specified elements and no others match as the specified logical criterion. It is possible to widen this criterion so that certain elements are allowed, but not required, using the `/OPTIONAL` and/or `/O_SPAN` qualifiers.

Use `/EXACT` with `/PEAKS` to specify that the error range specified for peak positions should not be extended, but instead be used as given. (See the description given for `/ERROR`.)

The following qualifiers may not be used with `/EXACT` and `/ELEMENTS`: `/CARDS`, `/NAME`, `/PEAKS`, `/OR`, `/AND`, `/ERROR`, `/FAST` `/LEVEL` or `/COUNT`.

The following qualifiers may not be used with `/EXACT` and `/PEAKS`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/FAST`, `/COUNT` `/OPTIONAL`, or `/O_SPAN`.

`/FAST` Use `/FAST` with `/PEAKS` to specify that the error range specified for peak positions may be extended for most efficient searching. (See the description given for `/ERROR`.)

The following qualifiers may not be used with `/FAST`: `/CARDS`, `/NAME`, `/ELEMENTS`, `/E_SPAN`, `/OPTIONAL`, `/EXACT`, `/COUNT` or `/O_SPAN`.

`/OR` Use `/OR` with either `/PEAKS` or `/ELEMENTS` to specify that any entry containing the specified element or peak is a match for the specified logical criterion.

The following qualifiers may not be used with `/OR`: `/CARDS`, `/NAME`, `/AND`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`. Also, if `/ELEMENTS` and `/OR` are used, `/EXACT` cannot be used.

`/AND` — Use `/AND` with either `/PEAKS` or `/ELEMENTS` to specify that only entries containing all of the specified elements or peaks match for the specified logical criterion.

The following qualifiers may not be used with `/AND`: `/CARDS`, `/NAME`, `/OR`, `/COUNT`, `/OPTIONAL`, or `/O_SPAN`. Also, if `/ELEMENTS` and `/AND` are used, `/EXACT` cannot be used.

`/OPTIONAL=optional_list`
`/O_SPAN=opt_range(s)` — Use `/OPTIONAL` or `/O_SPAN` with `/ELEMENTS` to specify that only entries containing all of the required elements specified in the `required_list` (see `/ELEMENTS` and `/E_SPAN`) and optionally those in the optional_list, but no others, as the specified logical criterion. `/O_SPAN` is equivalent to `/OPTIONAL` except that ranges of elements may be specified.

Examples of the use of this qualifier are:

`/OPTIONAL=SI`

`/ig=(si,o,H)`

`/O_SPAN=(H,BE)`

`/O_SPAN=(BE,H)` (equivalent to previous)

`/OPTIONAL=(H,HE,LI,BE)` (equivalent to previous)

`/O_SPAN=(H,BE,C,F)` specifies two ranges: from H to Be and from C to F.

Note that capitalization is ignored and the elements must be surrounded by parentheses and separated by commas, if more than one element is specified. Ranges may be specified in either ascending or descending order. To specify more than one range, specify more than one pair of endpoints.

The following qualifiers may not be used with `/OPTIONAL` or `/O_SPAN`: `/CARDS`, `/NAME`, `/PEAKS`, `/FAST`, `/OR`, `/AND`, `/ERROR`, `/COUNT`, or `/LEVEL`. Qualifier `/EXACT` is assumed to be present if `/OPTIONAL` or `/O_SPAN` is used and thus is optional. `/O_SPAN` may be used with `/OPTIONAL`.

2.12 Command READ

Reads a table (subfile) written by the WRITE command, prepared using some other program, such as MATCH, or one of the standard ICDD-JCPDS subfiles. The READ command can also be used to read a list of entries from a free-format ASCII text file or to select a list of entries in a range by number.

PARAMETER

`file_name` — A single file may be specified on the command line containing the name of the file to be read. If the file is not specified, a prompt will be given to request a file name to be read.

If no file extension is supplied, the default extension is `.USRPDF`

To read one of the standard subfiles, omit the `file_name` parameter and specify the `/SUBPDF` qualifier.

QUALIFIERS

`/SUBPDF=sub_file` Use this option to read in one of the standard subfiles, such as the the inorganic subfile.

The available subfiles are:

FULL	all entries in the database
NULL	null table (a table without any entries)
INORGANICS	Inorganic materials
ORGANICS	Materials with a C-H bond
COMMON	commonly found materials or phases
MINERALS	Minerals, natural and synthetic
METALS	metals, alloys and related materials
NIST	patterns recorded by NIST (NBS)
FORENSIC	materials of forensic interest
ZEOLITES	zeolites and molecular sieves
DELETED	superceeded but not removed patterns (if any)
LOCAL	locally defined patterns (if any)
SUPERCON	superconductors and related materials
EXPLOSIVES	explosives and related materials
EDUCATION	educationally relevant materials
CEMENT	materials related to cement production
CORROSION	corrosion products and related materials

Note that the `sub_file` name may be abbreviated by only including the initial letters as long as the name is uniquely specified. Also, note that by default, "DELETED" patterns are not included, unless the `DELETE/INCLUDE` command is used to force inclusion of deleted patterns.

Do not include a `file_name` parameter if `/SUBPDF` is used.

`/LIST=list_file` Use this option to read a list of entries from a text file, named `list_file` (with default extension `.CARDS`). This file will usually be prepared prior to starting LOGIC through use of a text editor or with a non-Powder Suite program. The `list_file` contains a list of ICDD-JCPDS entries with one entry entry per line in the file. If an invalid number is used, a warning is reported. The entry number may entered either with or without a comma separating the set number from the entry number (38,1 and 380001 are equivalent). Comments may be included on each line provided that two commas or are placed before the comment or the comment starts after column 20 (see below). Blank lines in the file are ignored. A negative set number terminates reading the file, but use of a -1 is not required.

Sample `list_file`:

```
        380001,,        this is the 1st entry in the list

        390001,,        this is the last entry
        -1
```

The `/LIST` option may not be used with `/SUBPDF` or `/RANGE`. Omit the `file_name` parameter if `/LIST` is used.

`/RANGE=(entry1,entry2)` Create a list with entries starting with `entry1` and ending with `entry2`. The number must contain both the set and entry numbers. For example `READ/RANGE=(360000-369999)` will select all entries in set 36. The `/RANGE` option may not be used with `/SUBPDF`, `/LIST`. Omit the `file_name` parameter if `/RANGE` is used.

`/OR` Specify this option to merge the requested subfile with the current table. Thus, the new current table will contain the entries in either the subfile OR the current table. (`NEW_TABLE = OLD_TABLE .or. SUB_FILE`)

`/OR` may not be used with `/AND`, `/NOT` or `/REPLACE`

`/AND` Specify this option to match the requested subfile against the current table. The new current table will contain the entries in both the subfile AND the current table. (`NEW_TABLE = OLD_TABLE .and. SUB_FILE`)

`/AND` may not be used with `/OR`, `/NOT` or `/REPLACE`

`/NOT` Specify this option to cull entries from the requested subfile from the current table. All entries present in the both subfile and the current table will be removed from in the new current table. (`NEW_TABLE = OLD_TABLE .and. .not. SUB_FILE`)

`/NOT` may not be used with `/OR`, `/AND` or `/REPLACE`

`/REPLACE` Specify this option to set the new current table to be the same as the requested subfile. (`NEW_TABLE = SUB_FILE`)

`/REPLACE` may not be used with `/OR`, `/AND` or `/NOT`

2.13 Command TABLES

Prints a table of the d-spaces and chemical name for all entries in the current list on the PS hardcopy listing device. If the wavelength has been set (see command WAVELENGTH), both d-spaces and 2θ angles are printed. (See the descriptions of the `PS_HDEV` and `PS_HCOM` logical names in the Installation Instructions chapter.)

QUALIFIERS

`/FULL` If this qualifier is used, the full ICDD-JCPDS (PDF-2) entry is displayed.

2.14 Command WAVELENGTH

Peaks positions may be input or output as d-spacings (in Å) or as 2θ (Bragg) angles corresponding to a given x-ray or neutron wavelength. This command is used to select between d-spacings and angles and to select a wavelength for the latter option.

The current mode of the program is displayed in the header line at the top of the computer screen; the default when the program is started is d-space mode.

PARAMETER

`wave_length`	A single wavelength value may be specified directly, where `wave_length` is the x-ray or neutron wavelength in Å. (The `target_type` will be assumed to be `SY` for synchrotron radiation). If `0.0` is used for the `wave_length`, the program will enter d-space mode (same as specifying `WAVELENGTH/NOTARGET`). If `wave_length` is used, `/TARGET` and `/WTYPE` should not.

QUALIFIERS

`/TARGET=target_type`
`/TARGET`
`/NOTARGET`
	Specifies an x-ray target for conventional x-ray sources. The choices for targets are: `Cu`, `Mo`, `Ni`, `Co`, `Fe`, `Cr`, `Ag`, `NU`, or `SY`. Specifying `/TARGET` without a `target_type` is equivalent to `/TARGET=CU`. (Capitalization of the target type is ignored.)
	
	If `NU` or `SY` (for neutron or synchrotron radiation) is used, the program prompts for a wavelength.
	
	For input/output using d-spacings specify `/NOTARGET`
	
	The `/TARGET` option cannot be specified with a `wave_length` value.

`/WTYPE=wave_type`	`wave_type` may be either 1, 2 or 3 which determines the exact value used for the wavelength specified with `/TARGET`. The choices are: 1 to use $K\alpha_1$ radiation 2 to use $K\alpha_2$ radiation 3 to use the intensity weighted average of $K\alpha_1$ and $K\alpha_2$ radiation. Specifying `/WTYPE` without a value for `wave_type` is equivalent to specifying `/WTYPE=1`. This qualifier is ignored if the radiation source has a single wavelength, (e.g. `/TARGET=NU` or `/TARGET=SY`) or a `wave_length` value is specified.

EXAMPLES

`WAVELENGTH/TARGET=CU/WTYPE=3`
The wavelength will be set to the average of Cu Kα_1 and Kα_2.

`WAVELENGTH/TARGET` The wavelength will be set to Cu Kα_1

`WAVE/NOTAR` Peaks positions, etc. will be displayed as d-spaces.

`WAVE 0.0` Peaks positions, etc. will be displayed as d-spaces.

`WAVE 2.5401` The wavelength will be set to 2.5401Å.

`WAVE` The user will be prompted to choose a wavelength or two use d-spacings.

`WAVELENGTH/TARGET=NU/WTYPE=3`
The user will be prompted to enter a wavelength; the `/WTYPE=3` qualifier will be ignored.

2.15 Command WRITE

This command writes the current list in a format suitable for use as a "user supplied" PDF subfile for program MATCH.

PARAMETER

`file_name` A single file may be specified on the command line containing the name of the file to be written. If the file is not specified, a prompt will be given requesting a file name to be written.

If no file extension is supplied, the default extension is `.USRPDF`

EXAMPLES

`WRITE MYINDEX.FILE` This writes file `MYINDEX.FILE` on the current default device and directory.

`WRITE XRAY:[mother.group]myindex`
This writes file `[MOTHER.GROUP]MYINDEX.USRPDF` on device `XRAY`.

`WRITE` The program will prompt for the name of a file to write.

2.16 Logic Examples

A few examples are presented to show how LOGIC may be used. Note that there may be several ways to achieve the same results [as is shown in in Example 1(a) and (b).] Also note that the `READ` and `WAVELENGTH` commands may not be needed, as the subfile may be selected when the program starts and the wavelegth may have already been set appropriately.

Example 1(a):

Find all entries in the full database that contain both Si and O and may also contain Al and/or H (or neither) The resulting entries are then examined using the `BROWSE` command.

```
READ/REPLACE/SUBPDF=FULL\_JCPDS
MATCH/ELEMENT=(SI,O)/OPTIONAL=(AL,H)
BROWSE
```

Example 1(b):

Find all entries in the full database that contain both Si and O and may also contain Al and/or H (or neither). This yields the same results as Example 1(a).

```
READ/REPLACE/SUBPDF=NULL
MATCH/ELEMENT=(SI,O)/OPTIONAL=(AL,H)
BROWSE
```

Example 2:

Find all entries in the metals section of database that contains Fe or Mn and two or three other elements. The entries must have a 30% or greater intensity peak within approximately 0.25 degrees of 12, 14 or 16 degrees and may not have any strong peaks (greater than 70%) between approximately 5 and 10 degrees. (Angles are 2θ values for Cu Kα_1 radiation).

Two lisings of these entries are made, one with the entry numbers and the other with the most intense three lines permuted and sorted. The first list will be printed and the second list will be displayed on the screen and then optionally printed.

```
READ/REPLACE/SUBPDF=METAL
MATCH/ELEMENT=(FE,MN)/OR
WAVELENGTH/TARGET=CU/WTYPE=1
MATCH/PEAK=(12,14,16)/OR/ERROR=0.25/LEVEL=70/FAST
CULL/PEAK=7.5/ERROR=2.5/LEVEL=30/FAST
INDEX/NAME/PRINT
INDEX/HANAWALT=3
```

Example 3:

For some complex searches, it may be necessary to perform a search in sections and save intermediate results on files and finally combine these files. To find all the entries in the ZEOLITE database that contain C plus all the entries in the ORGANIC database that contain both Al and Si, it is necessary to perform each search separately.

```
READ/REPLACE/SUBPDF=ZEOLITE
MATCH/ELEMENT=(C)/OR
COMMENT Carbon containing Zeolites
WRITE c-zeol
READ/REPLACE/SUBPDF=ORGANIC
MATCH/ELEMENT=(AL,SI)/AND
COMMENT Alumino-silicate organics
READ/OR c-zeol
COMMENT C-containing Zeolites and Al-Si organics
```

2.17 Sample LOGIC Run

The following section shows the output from program LOGIC in response to the commands in Example 1(b), above. The sequence in the example is repeated twice, first where commands are input with all needed qualifiers and parameters. In the second case, no qualifiers or parameters are specified and the program prompts to select options and request values.

Computer output is shown in `this typestyle`, while user responses are given in *italics*; <*CR*> indicates where the Return (or Enter) key has been pressed without other input to select the default response.

```
Welcome to the POWDER SUITE

Available Options Are:
HELP, LOGIC, SEARCH, INIT, EXIT
ENTER OPTION> logic
Welcome to program LOGIC.

Copyright 1988-1990 by Brian H. Toby and E. I. du Pont de Nemours and Co.
JCPDS database Copyright 1990 by the International Centre for Diffraction Data

Select a starting subfile:
   (0)  Full JCPDS database (default)
   (1)  Inorganic subfile
   (2)  Organic subfile
   (3)  Common phases subfile
   (4)  Minerals subfile
   (5)  Metals and alloys subfile
   (6)  NIST patterns subfile
   (7)  Forensic materials subfile
   (8)  Zeolite subfile
   (9)  Deleted Patterns subfile
  (10)  Locally entered subfile
  (11)  Null (empty) subfile
  (12)  User supplied subfile
  (-1)  Enter and display JCPDS card(s) by number
Choose an option by number [Default=0]: <CR>

The current table contains 53010 hits, out of 57981

Press RETURN to continue
-----------------------------------------------------------------------
 LOGIC v3.1                           No Deleted               D-space
-----------------------------------------------------------------------

                                                NUMBER OF PHASES: 53010
Current LOGIC List:
   1) DELETED/EXCLUDE
   2) Starting with Full JCPDS database (w/o deleted entries)
Enter a LOGIC command (or HELP)
LOGIC> read/rep/sub=null

File "Null (empty) subfile" contains     0 hits, out of 57981

Press RETURN to continue
-----------------------------------------------------------------------
 LOGIC v3.1                           No Deleted               D-space
```

```
----------------------------------------------------------------------
                                                NUMBER OF PHASES:     0
Current LOGIC List:
   1) DELETED/EXCLUDE
   2) READ/REPLACE file: "Null (empty) subfile"
Enter a LOGIC command (or HELP)
LOGIC> add/elem=(si,o)/opt=(al,h)

There are    98 hits corresponding to logic:
   /ELEMENTS=(O,Si)/EXACT/OPTIONAL=(H,Al)
...After removing deleted entries there are   75 hits

Current Table contains     0 hits, out of 57981
After the ADD operation, the Table will contain    75 hits

Proceed with change to table? (Y/N) [default=Y]: <CR>
----------------------------------------------------------------------
 LOGIC v3.1                         No Deleted              D-space
----------------------------------------------------------------------
                                                NUMBER OF PHASES:    75
Current LOGIC List:
   1) DELETED/EXCLUDE
   2) READ/REPLACE file: "Null (empty) subfile"
   3) ADD/ELEMENTS=(O,Si)/EXACT/OPTIONAL=(H,Al)
Enter a LOGIC command (or HELP)
LOGIC> browse
Initializing PDF-2 database

Opening the PDF-2 disk file PUBLIC_DISK:[PS.SET40]JCPDS.DIRECT;1

Press return to sequence though the phases
+n   to skip ahead by "n" phases,
-n   to skip backward by "n" phases,
>n   to skip to entry number "n",
[crd to skip to JCPDS entry "crd",
C    to Cull (remove) current entry from table,
P    to Print current entry SUMMARY and advance to next,
D    to Display all data on the current entry,
A    to print All data on the current entry,
^Z or E to return to the main menu
(Commands:+n,-n,>n,[c,^Z=exit,?=help) press return for phase #1: <CR>

[090451]     I/Ic=  0.00E+00  QM=                    Phase 1 of 75
         Al2 Si2 O5 ( O H )4 !2 H2 O
         ALUMINUM SILICATE HYDROXIDE HYDRATE / HALLOYSITE-10A
 10.099  90
  4.420 100
  3.340  90
  2.560  80
  2.360  60
  2.230  20
  2.060  10
  1.678  80
  1.481  90
  1.283  70
  1.232  70
```

```
  1.105  40
  1.021  20
  0.963  20
  0.855  40
  0.838  20
(Commands:P,C,+n,-n,>n,[#,D,A,^Z=exit,?=help) Phase #1/75> <CR>

[090453]     I/Ic=  0.00E+00  QM=                     Phase 2 of 75
         Al2 Si2 O5 ( O H )4
         ALUMINUM SILICATE HYDROXIDE / HALLOYSITE-7A
  7.499  90
  4.420 100
  3.630  90
  2.560  80
  2.360  60
  2.230  20
  2.060  10
  1.678  80
  1.481  90
  1.283  70
  1.232  70
  1.105  40
  1.021  20
  0.963  20
  0.855  40
  0.838  20
(Commands:P,C,+n,-n,>n,[#,D,A,^Z=exit,?=help) Phase #2/75> <CR>

[100446]     I/Ic=  0.00E+00  QM=i                    Phase 3 of 75
         Al2 Si2 O5 ( O H )4
         ALUMINUM SILICATE HYDROXIDE / DICKITE-2MT2M#1\RG
  7.150 100      2.326  90
  4.460  40      2.212  20
  4.438  40      2.106  10
  4.366  40      2.025   5
  4.267  30      1.975  50
  4.124  70      1.937  10
  3.961  20      1.898  20
  3.799  60      1.859  30
  3.580 100      1.805  10
  3.430  30      1.785  10
  3.262  20      1.762   5
  3.099  20      1.720  10
  2.938  20      1.686  10
  2.796  20      1.652  50
  2.562  20      1.613  10
  2.556  20      1.586  10
  2.528   5      1.555  40
  2.510  50      1.508   5
  2.411   5      1.489  50
  2.386  10
(Commands:P,C,+n,-n,>n,[#,D,A,^Z=exit,?=help) Phase #3/75> d

10-446                JCPDS-ICDD Copyright 1990                  QM= i
Al Si O (OH)
  2  2 5    4

Aluminum Silicate Hydroxide                                Dickite-\IT2M#1\RG
--------------------------------------------------------------------------------
Rad:     CuKa  Lambda: 1.5418         Filter: Ni           d-sp: D.S. -114.6
```

```
Cutoff:          Int: Visual              I/Icor:
Ref: Newnham, Brindley, Private Communication
------------------------------------------------------------------------------
Sys: Monoclinic             S.G.: Cc (9)
a: 5.149           b: 8.949          c: 14.419          A:          C:
A:                 B: 96.80          C:                 Z: 4     mp:
Ref: Newnham, Brindley, Acta Crystallogr., 9 759 (1956)
Dx:  2.60     Dm:           SS/FOM: F(30)=27.9(.0179,60)
------------------------------------------------------------------------------
ea: 1.565      nwB: 1.566       ey: 1.568       Sign: +    2V: 73 deg.
Ref: Newnham, Thesis, P., Pennsylvania State Univ., University Park,
Pennsylvania, USA., Private Communication
Enter N or <CR> for Next pg; P for Previous; E to Exit <CR>

10-446                JCPDS-ICDD Copyright 1990                    QM= i
Color: Colorless
Dickite from Schuylkill, Pennsylvania, USA.  Bailey [Am. Mineral.,
48 1196, (1963)] proposes new setting with a, b, as above, c=14.736,
beta=103 deg.35; gives fully indexed powder pattern.  Intensities verified by
calculated pattern.  Other data 10-430.  Kaolinite-Serpentine group,
dioctahedral subgroup.  C.D. Cell: a=14.419, b=8.949, c=5.149, beta=96.80,
a/b=1.6112, c/b=0.5754, S.G.=Aa (9).  PSC: mC68.  Plus reflections to 1.126.
Mwt: 258.16.  Volume[CD]: 659.73.
Strong lines:  7.15/X  3.58/X  2.33/9  4.12/7  3.80/6  2.51/5  1.98/5  1.65/5
Enter N or <CR> for Next pg; P for Previous; E to Exit <CR>

10-446                JCPDS-ICDD Copyright 1990                    QM= i
 39 reflections in pattern.  Page 1 of 2.  Radiation=  1.54050
------------------------------------------------------------------------------
!   d A   ! Int.!        h k l         !   d A   ! Int.!        h k l         !
!---------+-----+----------------------+---------+-----+----------------------!
! 7.15    ! 100 !       0  0  2        ! 2.556   !  20 !       2  0  0        !
! 4.46    !  40 !       0  2  0        ! 2.528   !   5 !      -1  1  5        !
! 4.438   !  40 !       1  1  0        ! 2.510   !  50 !       1  3  1        !
! 4.366   !  40 !      -1  1  1        ! 2.411   !   5 !       0  2  5        !
! 4.267   !  30 !       0  2  1        ! 2.386   !  10 !       0  0  6        !
!         !     !                      !         !     !                      !
! 4.124   !  70 !       1  1  1        ! 2.326   !  90 !      -1  3  3        !
! 3.961   !  20 !      -1  1  2        ! 2.212   !  20 !       1  3  3        !
! 3.799   !  60 !       0  2  2        ! 2.106   !  10 !       0  2  6        !
! 3.580   ! 100 !       0  0  4        ! 2.025   !   5 !       0  4  3        !
! 3.430   !  30 !      -1  1  3        ! 1.975   !  50 !      -1  3  5        !
!         !     !                      !         !     !                      !
! 3.262   !  20 !       0  2  3        ! 1.937   !  10 !       2  2  3        !
! 3.099   !  20 !       1  1  3        ! 1.898   !  20 !       0  4  4        !
! 2.938   !  20 !      -1  1  4        ! 1.859   !  30 !       0  2  7        !
! 2.796   !  20 !       0  2  4        ! 1.805   !  10 !       2  2  4        !
! 2.562   !  20 !      -1  3  1        ! 1.785   !  10 !       1  1  7        !
------------------------------------------------------------------------------
Enter N or <CR> for Next pg; P for Previous; E to Exit; D/2/1/S/Q to convert <CR>
10-446                JCPDS-ICDD Copyright 1990                    QM= i
 39 reflections in pattern.  Page 2 of 2.  Radiation=  1.54050
------------------------------------------------------------------------------
!   d A   ! Int.!        h k l         !   d A   ! Int.!        h k l         !
```

```
!---------+-----+-------------------+---------+-----+--------------------!
! 1.762   !   5 !       0  4  5     !         !     !                    !
! 1.720   !  10 !      -1  1  8     !         !     !                    !
! 1.686   !  10 !      -3  1  1     !         !     !                    !
! 1.652   !  50 !      -1  3  7     !         !     !                    !
! 1.613   !  10 !      -1  5  3     !         !     !                    !
!         !     !                   !         !     !                    !
! 1.586   !  10 !      -2  2  7     !         !     !                    !
! 1.555   !  40 !      -2  0  8     !         !     !                    !
! 1.508   !   5 !       0  4  7     !         !     !                    !
! 1.489   !  50 !      -3  3  1     !         !     !                    !
--------------------------------------------------------------------------
Enter N or <CR> for Next pg; P for Previous; E to Exit; D/2/1/S/Q to convert <CR>
(Commands:P,C,+n,-n,>n,[#,D,A,^Z=exit,?=help) Phase #3/75> ^Z

--------------------------------------------------------------------
 LOGIC v3.1                          No Deleted             D-space
--------------------------------------------------------------------

                                                NUMBER OF PHASES:    75
Current LOGIC List:
   1) DELETED/EXCLUDE
   2) READ/REPLACE file: "Null (empty) subfile"
   3) ADD/ELEMENTS=(O,Si)/EXACT/OPTIONAL=(H,Al)
Enter a LOGIC command (or HELP)
LOGIC> read
Choose a (sub)file to read:
   (0)  Full JCPDS database (default)
   (1)  Inorganic subfile
   (2)  Organic subfile
   (3)  Common phases subfile
   (4)  Minerals subfile
   (5)  Metals and alloys subfile
   (6)  NIST patterns subfile
   (7)  Forensic materials subfile
   (8)  Zeolite subfile
   (9)  Deleted Patterns subfile
  (10)  Locally entered subfile
  (11)  Null (empty) subfile
  (12)  User supplied subfile
  (13)  Read a list of JCPDS cards from a file
  (-1)  Enter a range of JCPDS cards
Enter a number corresponding to the (sub)file: 11

File "Null (empty) subfile" contains     0 hits, out of 57981

Press RETURN to continue

--------------------------------------------------------------------
 LOGIC v3.1                          No Deleted             D-space
--------------------------------------------------------------------

                                                NUMBER OF PHASES:     0
Current LOGIC List:
   1) DELETED/EXCLUDE
   2) READ/REPLACE file: "Null (empty) subfile"
Enter a LOGIC command (or HELP)
```

```
LOGIC> add
The logical options are:
(1) ELEMENTS -- search by chemical composition
(2) CARDS    -- search by JCPDS card number
(3) PEAKS    -- search by angles/d-spaces
(4) COUNT    -- search by # of elements in material

Choose an option number: 1

Enter the chemical symbols for elements one per line (case will be ignored)
Enter a blank line when done.
ELEMENT> si
ELEMENT> o
ELEMENT> <CR>
Choose a logic type:
  (1) OR       -- materials with ANY of the selected elements
  (2) AND      -- materials with ALL of the selected elements
  (3) EXACT    -- materials with ALL of the selected elements
                  and no others
  (4) OPTIONAL -- same as EXACT but specified optional elements
                  may or may not be present
Enter your choice (default=2): 4
Enter the chemical symbol for elements to be ignored
OPTIONAL> al
OPTIONAL> h
OPTIONAL>

There are    98 hits corresponding to logic:
   /ELEMENTS=(O,Si)/EXACT/OPTIONAL=(H,Al)
...After removing deleted entries there are   75 hits

Current Table contains     0 hits, out of 57981
After the ADD operation, the Table will contain    75 hits

Proceed with change to table? (Y/N) [default=Y]: <CR>
-----------------------------------------------------------------------
 LOGIC v3.1                           No Deleted            D-space
-----------------------------------------------------------------------

                                                 NUMBER OF PHASES:    75
Current LOGIC List:
   1) DELETED/EXCLUDE
   2) READ/REPLACE file: "Null (empty) subfile"
   3) ADD/ELEMENTS=(O,Si)/EXACT/OPTIONAL=(H,Al)
Enter a LOGIC command (or HELP)
LOGIC> browse

Press return to sequence though the phases
+n   to skip ahead by "n" phases,
-n   to skip backward by "n" phases,
>n   to skip to entry number "n",
[crd to skip to JCPDS entry "crd",
C    to Cull (remove) current entry from table,
P    to Print current entry SUMMARY and advance to next,
D    to Display all data on the current entry,
A    to print All data on the current entry,
```

```
^Z or E to return to the main menu
(Commands:+n,-n,>n,[c,^Z=exit,?=help) press return for phase #1:  <CR>

[090451]     I/Ic=  0.00E+00  QM=                     Phase 1 of 75
         Al2 Si2 O5 ( O H )4 !2 H2 O
         ALUMINUM SILICATE HYDROXIDE HYDRATE / HALLOYSITE-10A
 10.099  90
  4.420 100
  3.340  90
  2.560  80
  2.360  60
  2.230  20
  2.060  10
  1.678  80
  1.481  90
  1.283  70
  1.232  70
  1.105  40
  1.021  20
  0.963  20
  0.855  40
  0.838  20
(Commands:P,C,+n,-n,>n,[#,D,A,^Z=exit,?=help) Phase #1/75> ^Z
```

Chapter 3: Program SEARCH

Program SEARCH is used to search the ICDD-JCPDS database to find known phases matching a diffraction pattern from an unknown materials, which may contain one or more phases.

When running program SEARCH, it is first necessary to set up the search by specifying the peak positions and the parameters which govern how the search will be performed. The `READ` command may be used to read in a peak/data file. As an alternative to supplying peak positions from a file, peak positions may be input using the `EDIT` command, which invokes the peak list editor. If SEARCH has previously been run, the previous peaks and parameters may be reloaded using command `LOAD`.

Search parameters may be modified using commands `SET`, `STARTFILE`, and `TITLE` and displayed using command `SHOW`. Peak positions and intensities may be modified using the `EDIT` command. Units for peak positions may be d-spaces or 2θ angles, as selected using the `WAVELENGTH` command. The inclusion of deleted patterns may be set using command `DELETED`.

After the search parameters have been set, the search is performed using command `SEARCH`, which is equivalent to entering commands `REDUCE`, `MATCH` and `REPORT`. ICDD-JCPDS entries which have been selected as potential "hits" are written onto a file which may be read by the LOGIC program. Command `LOGIC` starts this program and passes the file of "hits."

Other commands available within SEARCH are: `DCL`, `HELP`, `FILE`, `EXIT` and `QUIT`.

A search consists of four steps:

1 Setting the scope of the search – restricting the search to the entries in a ICDD-JCPDS subfile or by using chemistry to constrain the search (command `STARTFILE`);

2 Reducing the extent of the search by dropping entries that are unlikely to be "hits" (command `REDUCE`):

– by eliminating entries that do not have at least one strong peak matching one of the observed strong peaks ["Required Lines"];

– by eliminating entries that have a strong peak in reqions of the observed pattern where no significant intensity is present ["Forbidden Lines"];

3 Matching the remaining ICDD-JCPDS entries against the list of observed peaks – ICDD-JCPDS entries with too many unmatched peaks or not matching a sufficient number of observed peaks are dropped; the remaining entries are written as a user subfile (command `MATCH`);

4 Evaluating the "goodness of fit" between each remaining entries and the observed pattern – optionally, the remaining entries may be ranked and the entries with the best fits may also be written as a user subfile (command REPORT).

The `SEARCH` command performs steps 2, 3 and 4 and thus is equivalent to using the `REDUCE`, `MATCH` and `REPORT` commands sucessively. These steps must be performed in order, but any step may be omitted.

3.1 Command DCL

Spawns a subprocess to execute DCL commands, type LOGOUT to return back to SEARCH loss of the current work. This command is useful for quick DCL "errands" such as answering a mail message without exiting the program.

3.2 Command DELETED

Some of the entries in the database are marked as "deleted" by the editors of the database. If these entries are included in the database (using the ENCODE program, PDF1) it is possible to select that these entries will be included or excluded from the operations of this program.

This command causes logical name `PS_DELETED` to be set so that subsequent operations with the program and with other programs in the Powder Suite package will use the same option. The default mode for the program is `DELETED/EXCLUDE`. However, if desired the `PS_DELETED` logical name may be predefined (see customization instructions) to change the default.

QUALIFIERS

`/INCLUDE`	Specifies that deleted entries will be included in the logical operations.
`/EXCLUDE`	Specifies that deleted entries will be not be included in the logical operations.

3.3 Command EDIT

Used to edit the list of peaks. Peaks may be added, deleted or changed. This operation must be done interactively. Note that intensities may be input with an arbitrary scale, but will be normalized internally before use.

3.4 Command EXIT

Type EXIT (which can be abbreviated to EX) to exit from the program. Alternately, pressing Control Z (`^Z`) will also cause the program to exit. Either causes the current search information to be written onto a load file (see commands `SET/NAME` and `LOAD`.)

When the load file is written, logical device name `SEARCH_FILE` is defined as the name of the load file. If program SEARCH is restarted in the same login session, the file defined by `SEARCH_FILE` (if any) may be read.

3.5 Command FILE

Allows a series of commands to be input to the program from an external file. The file should be prepared before starting the program, or using the `DCL` command to invoke an editor.

PARAMETER

`file_name`	A single file may be specified on the command line containing the name of the file with commands. If the file is not specified, a prompt will be given to request a file name. If no file extension is supplied, the default extension is `.CMD`

3.6 Command HELP

Invokes the VAX/VMS online help facility for help on this program.

3.7 Command IGNORE

This command is used to display and modify the range of angles/d-spaces which are used when searching the ICDD-JCPDS database. The ranges that have been set to be ignored are called "excluded regions." Peaks in a ICDD-JCPDS entry which are located in an excluded region are ignored, e.g. their presence will not disqualify the entry in the `REDUCE` step, nor will they be counted as unmatched peaks. Similarly, observed peaks which fall inside an excluded area are not used for searching and are not counted toward the percentage of matched peaks.

Two common applications which require use of excluded regions are: (1) to insure that only peaks on ICDD-JCPDS entries within the observed 2θ region are used – the regions below and above the measured diffraction pattern should be excluded. (2) to account for interference from known or identified phases. For example, if silicon is used as an internal standard, the silicon peaks could obscure a peak from an unknown phase. Thus, the regions immediately surrounding the silicon peaks should be treated as unknown and thus should be excluded from consideration.

Qualifier `/EXCLUDE` is used to add or increase the size of an excluded region and `/INCLUDE` is used to reset a region so that it is no longer excluded. Qualifier `/PEAK` is used to specify peaks to be excluded and qualifier `/RANGE` is used to a region to exclude/include. Alternately, qualifier `/CARD` is used to exclude all peaks in a ICDD-JCPDS entries above a threshold intensity. Qualifier `/DISPLAY` is used to display the current list of excluded regions.

When a raw datafile is read into this program, regions outside the range of the collected data are excluded. If a list of peaks is read from a peak file without a datafile, the regions below the lowest angle and above the highest angle are excluded. These excluded ranges may be extended using `/EXCLUDE` and reduced using `/INCLUDE`.

`/DISPLAY`
: Qualifier `/DISPLAY` produces a listing of the current "excluded regions". If this qualifier is combined with other qualifiers, the excluded regions will be displayed after any changes.

`/CARD=jcpds_card`
`/CARD`
: Qualifier `/CARD` excludes regions surrounding a ICDD-JCPDS entry. If supplied, `jcpds_card` is the 5 or 6 digit ICDD-JCPDS set and entry number (e.g. `/CARD=110011`). The width of the region around each peak may be specified using qualifier `/WIDTH` and the intensity threshold for ignored peaks may be specified using `/IMIN`. Qualifier `/CARD` cannot be used with `/INCLUDE` or `/EXCLUDE`.

`/IMIN=min_inten`
: `/IMIN` specifies the minimum intensity for ICDD-JCPDS peaks which will be "excluded". Peaks with relative intensity below `min_inten` (in units of % of the most intense peak) will not be used. Qualifier `/IMIN` cannot be used with `/INCLUDE` or `/EXCLUDE`.

`/INCLUDE` Specifies that the region or list of peaks (see `/RANGE` and `/PEAK`) will be reset so that these areas will be used in (will not be "excluded" from) the search.

Note that if `/CARD` has been used previously, all peaks that lie in the region to be included will be no longer be excluded.

Qualifier `/INCLUDE` cannot be used with `/CARD` or `/EXCLUDE`.

`/EXCLUDE` Specifies that the region or list of peaks (see `/RANGE` and `/PEAK`) will be set so that these regions will be "excluded" from the search.

Qualifier `/EXCLUDE` cannot be used with `/INCLUDE` or `/CARD`.

`/PEAK=position_list`
`/PEAK` Specifies a list of regions to be excluded or included in the search (see `/EXCLUDE` and `/INCLUDED`). The positions are the approximate centers of the regions; the length of each region will depend on the value of `DEL_2THETA` (see `/WIDTH`.)

More than one position may be specified by enclosing the list in parentheses and separating the points by commas, e.g.

`/PEAK=4.0` or

`/PEAK=(4.0,6.0)`

The units for `position_list` will be d-spaces in Å, unless a wavelength has be set, in which case the units will be degrees 2θ at the current wavelength.

Qualifier `/PEAK` cannot be used with `/RANGE` or `/CARD`.

`/WIDTH=D_2THETA` `D_2THETA` defines the half width to be allowed around a position specified using the `/EXCLUDE` or the `/INCLUDE` qualifiers or the ICDD-JCPDS peaks from a entry specified using the `/CARD` qualifier. The units for `D_2THETA` are degrees 2θ for Cu Kα_1 radiation. `D_2THETA` may be a floating point number.

`/RANGE=(min,max)`
`/RANGE` Specifies a single regions to be excluded or included in the search (see `/EXCLUDE` and `/INCLUDED`) by specifying an upper and lower limit. The limits must specified by as a list inside parentheses and separated by commas, e.g.

`/RANGE=(4.0,6.0)`

The units for `position_list` will be d-spaces in Å, unless a wavelength has be set, in which case the units will be degrees 2θ at the current wavelength.

Qualifier `/RANGE` cannot be used with `/PEAK` or `/CARD`.

3.8 Command LOAD

This command is used to reload the output file ("load file") from a previous run of SEARCH so that parameters may be easily changed. Thus the search run may quickly repeated with a new set of parameters, allowing the widening of a search that failed to find any matching phases or narrowing of a search that yielded too many unlikely matches.

The "search name" (see command `SET /NAME`) is set as the name of the LOAD file, after dropping the file extension, if one has been supplied.

PARAMETER

`file_name` A single file may be specified on the command line containing the name of the file to be read. If the file is not specified, a prompt will be given requesting a file name to read.

The default file extension for the "load file" is `.SEA_IN`.

3.9 Command LOGIC

This command causes the SEARCH run to be terminated and program LOGIC to be started. The results from the most recent search will be passed to program LOGIC. The program will save the current SEARCH parameters on a load file for future use before transferring control to program LOGIC.

3.10 Command MATCH

This command causes the program to invoke the `MATCH` step in the search procedure. In this step peaks in the observed pattern are compared line-by-line to the peaks in each possible hit remaining after the `REDUCE` step (or in the starting subfile, if the `REDUCE` step will be omitted). If the positions of two peaks (as 2θ values for $CuK\alpha_1$) agree within `DEL_2THETA`, the peaks are considered to "match" (see `SET/ERROR`).

For a JCPDS-ICDD entry to be retained by the `MATCH` step as a "hit" all but `DB_max_miss` of ICDD-JCPDS peaks above `DB_min_int` percent relative intensity must be matched (see `SET/DB_IMIN` and `SET/MAXDBMISS`). Also, at least `OBS_min_lines` percent of the lines above `OBS_min_int` percent relative intensity must be matched (see `SET/MATCHOBS` and `SET/OBS_IMIN`.

3.11 Command QUIT

Type QUIT to exit from the program without writing a load file or updating logical name `SEARCH_FILE`.

3.12 Command READ

Reads a list of peak positions and optionally a raw data file. Peaks in the peak list that are assigned to the Kα_2 wavelength will be ignored all others will be converted to d-spaces.

The "excluded regions", the ranges of d-spaces which are ignored during searching, are reset by the READ command. (See command `IGNORE` for more information about excluded regions). If peaks are input without a data file, the regions of d-spaces outside the range of peaks will be excluded. If a diffractogram is input as well, the regions outside the range of collected data will be excluded rather than the range of the data points (the collected data will usually cover a signifcantly larger region than the range of peaks). If the diffractogram will be used for FOM computations (see `SET/FOM` and `REPORT`), the background should be subtracted, prior to reading it in to SEARCH.

The search name is defined from the peak file name (including the device and directory if specified), but the file extension is dropped. This file name is used to define the names of the "load file," which is used for temporary storage of the current SEARCH settings; the "search output file," which will contain a user subfile created with the matches from the search; a "search report," if command `REPORT` is used to prioritize the matches; and a "starting subfile," if the `STARTFILE` command is used to spawn program LOGIC to create a subfile to narrow down the search using chemistry. See information on the `SET /NAME` subcommand, for more information on file naming.

See the section on File Formats in the first chapter for more information on formats for peak and data files.

PARAMETER

`file_name` A single file may be specified on the command line containing the name of the file to be read. If the file is not specified, the program will prompt for a file name to read.

It is usually preferable to supply the file name without a file extension, as the default extension will then depend on the file format. This improves the speed that the program has available when searching for the file. The subroutines which read data and peak files, (subroutines `READDATA` and `READPEAK` respectively), will attempt to determine the format of the file from the file contents and the extension.

QUALIFIER

`/FORMAT=fileform` This optional qualifier may be used to specify the file format that will be used for reading the file. (See the information on File Formats for the `fileform` codes). In most cases it is not necessary to specify the file format, as the program will discern the file format from the file. However, in certain cases where problems are encountered, it may be necessary to use the format option.

3.13 Command REDUCE

This command causes the program to reduce the number of ICDD-JCPDS entries that will be considered during the search by dropping entries that are unlikely to be "hits" by performing two screening steps:

- entries are eliminated if they do not have at least one strong peak matching one of the observed strong peaks ["Required Lines"];
- entries are eliminated if they have a strong peak in reqions of the observed pattern where no significant intensity is present [Forbidden Lines];

The screening steps improve the speed of searching the database because they use the bitmap indices to eliminate rapidly from consideration entries that cannot match the observed pattern.

The "Required Lines" screening step is governed by variables `Req_Index`, `R_Imin` and `DEL_2THETA`, which are changed using command `SET` (see qualifiers `/R_INDEX`, `/Rmin` and `/Error`). This step looks up each peak in the observed pattern above `R_Imin`% relative intensity in a peak index file selected by `Req_Index`. The peak positions in observed pattern and database must be within `DEL_2THETA` to match. Thus, patterns which do not have an observed peak matching some peak in the JCPDS-ICDD database within `DEL_2THETA` will be eliminated from further consideration as a potential match. This screening step may be skipped, if desired, by setting `Req_Index` to a value of 100 or greater.

The "Forbidden Lines" screening step is governed by variables `Forbid_Index`, `F_Imin` and `DEL_2THETA`, which are changed using command `SET` (see qualifiers `/F_INDEX`, `/Fmin` and `/Error`). This step elminates from further consideration entries in the JCPDS-ICDD database that have strong peaks where no intensity has been observed. The peak index selected by `Forbid_Index` is searched for peaks in the regions of the observed pattern where there are no peaks above `F_Imin`/intensity within `DEL_2THETA` and that have not been "excluded". Any JCPDS-ICDD entry with a peak in one of these regions will be eliminated from further consideration as a potential match. This screening step may be skipped, if desired, by setting `Forbid_Index` to a value of 100 or greater.

The `REDUCE` command need not be used, but if it will be used it must be specified before `MATCH` (or `REPORT`, if `MATCH` will also be omitted.) Command `SEARCH` performs the `REDUCE`, `MATCH` and `REPORT` steps sequentially.

3.14 Command REPORT

Used to print a report on the matches from the previous search and/or creates a graph with the observed pattern and likely matching patterns. If the `MATCH` step was not performed first, the report may be run using all entries in the current subfile (or those remaining after removing entries in the `REDUCE` step). Note that the REPORT step is usually rapid, but may take several minutes if more than a thousand entries will be considered.

For each entry, if two or more peaks match the observed pattern, three or four figures of merit (FOM) are computed based on how close the patterns match. The angle FOM reflects the descrepancies between matching observed and ICDD-JCPDS peak positions; the intensity FOM reflects the descrepancies between matching observed and ICDD-JCPDS peak intensities; a full-pattern FOM is computed if a raw data file is input to this program; the overall FOM is computed from the above FOM values.

The formulae used for FOM computation are:

$$\mathrm{FOM_I} = \frac{1}{\mathrm{n}} \sum \frac{|\mathrm{I_{obs}} - \mathrm{I_{JCPDS}}|}{\mathrm{I_{obs}} + \mathrm{I_{JCPDS}}}$$

$$\mathrm{FOM_D} = \sqrt{\frac{\mathrm{n} \sum \Delta\mathrm{A}^2 + \left(\sum |\Delta\mathrm{A}|\right)^2}{\mathrm{n}(\mathrm{n}-1)}}$$

$$\mathrm{FOM_{FP}} = \frac{1}{\sum \mathrm{I_{JCPDS}}} \sqrt{\sum \mathrm{I_{JCPDS}} - \mathrm{I_{raw}} \frac{\sum \mathrm{I_{raw}}}{\sum \mathrm{I_{JCPDS}}}}$$

Where n is the number of matched peaks, m is the number of missed peaks, ΔA is 100 times the closest JCPDS and observed peak positions in degrees 2θ at Cu $\mathrm{K}\alpha_1$. Where $\mathrm{I_{JCPDS}}$ and $\mathrm{I_{obs}}$ are the JCPDS and observed peak intensities, respectively and $\mathrm{I_{raw}}$ is the intensity of the raw, background subtracted pattern at the specified position.

The formula used for the overall FOM depends on the setting for `Calc_type` (see command `SET/FOM`).

`Calc_type = 0`

$$\mathrm{FOM_{overall}} = \mathrm{FOM_D}\,\mathrm{FOM_I} \left(\frac{\mathrm{n}+\mathrm{m}}{\mathrm{n}}\right)^2 \sqrt{\frac{\mathrm{n_{obs}}}{\mathrm{n}}}$$

`Calc_type = 1`

(differences between observed and JCPDS peak intensities do not affect the overall FOM.)

$$\mathrm{FOM_{overall}} = \mathrm{FOM_I} \left(\frac{\mathrm{n}+\mathrm{m}}{\mathrm{n}}\right)^2 \left(\frac{\mathrm{n_{obs}}}{\mathrm{n}}\right)$$

`Calc_type = 2`

(differences between matching observed and ICDD-JCPDS peak positions do not affect the overall FOM.)

$$\mathrm{FOM_{overall}} = \mathrm{FOM_D} \left(\frac{\mathrm{n}+\mathrm{m}}{\mathrm{n}}\right)^2 \sqrt{\frac{\mathrm{n_{obs}}}{\mathrm{n}}}$$

`Calc_type = 3`

$$\mathrm{FOM}_{\mathrm{overall}} = \mathrm{FOM}_{\mathrm{FP}}.$$

Following the computation of the FOM values and the optional sort step, it is possible to display stick diagrams for the matching patterns along with the observed peaks or the observed diffractogram for each pattern. Patterns will be displayed by order of FOM, if sorted.

The graphical display shows the observed peaks or diffractogram and an adjustable number of "hits." At the bottom of the page, the excluded regions of the pattern and the "forbidden" regions of the pattern are shown as two lines. If the graphics device supports display of more than one color on the screen. Different colors will be used to show excluded peaks. Otherwise, different line styles will be used.

QUALIFIERS

`/PRINT`	Causes the report to be printed rather than displayed first on the terminal.

3.15 Command SEARCH

This command causes the program to invoke the search procedure. The search may be performed interactively or in batch mode. If batch mode is selected, a load file will be written, a batch job will be submitted and the program will then exit. The `SEARCH` command performs the equivalent of the following three commands: `REDUCE`, `MATCH` and `REPORT`

QUALIFIERS

`/BATCH`	This option causes the search to be performed in batch mode.
`/INTERACTIVE`	This option causes the search to be performed interactively.
`/PRINT`	Causes the report to be printed rather than displayed first on the terminal. Ignored if used with the `/BATCH` option.

3.16 Command SET

This command is used to set parameters which govern the search. If SET is called with one or more qualifiers, the specified parameters are updated and no prompts are generated. However, if SET is used with no qualifiers, prompts are generated which allow all parameters to be updated.

When the search is performed (commands `REDUCE`, `MATCH` and `REPORT`), peak positions from each appropriate entry in the ICDD-JCPDS database are compared to positions from the list of peaks in the observed pattern. Two peaks are considered to "match", if the 2θ values agree within `DEL_2THETA` (see `/ERROR`).

In the `MATCH` step, observed and database entries are compared peak-by-peak. If no observed peak matches for a ICDD-JCPDS peak and the relative intensity of that peak is above `DB_min_int` percent, (see `/DB_IMIN`), the peak is counted as a "miss." If more than `DB_max_miss` ICDD-JCPDS peaks are not "missed"(see `/MAXDBMISS`), the entry will be rejected. Also in the `MATCH` step, the number of peaks in the observed pattern which have been matched to ICDD-JCPDS are also counted. If fewer than `OBS_min_lines` percent of the total observed peaks above `OBS_min_int` percent relative intensity are matched, the entry is rejected. Note that an observed peak may be matched by several ICDD-JCPDS lines, and a ICDD-JCPDS line can be matched by several observed peaks.

The speed of the search is improved through three optional steps. The first is by restricting the search to a ICDD-JCPDS or user subfile created in program LOGIC (see command `STARTFILE`). The other two methods utilize the strong peak indices to eliminate entries quickly which have strong peaks where no intensity is observed (see `/F_INDEX` and `/Fmin`, below) and/or to restrict the search to entries having at least one strong line matching the an observed line in the pattern (see `/R_INDEX` and `/Rmin`, below). The strong peak choices are utilized in the `REDUCE` step, thus these parameters are ignored unless either command `REDUCE` or `SEARCH` is used.

QUALIFIERS

`/Error=DEL_2THETA`

`DEL_2THETA` defines the allowed discrepancy between peak positions in the observed pattern and those in the database used in the `MATCH` and `REPORT` steps. These steps match the peak positions using peak positions transformed to angles for Cu Kα_1 radiation. Thus, `DEL_2THETA` defines a discrepancy in units of degrees 2θ for Cu Kα_1 radiation, regardless of the wavelength mode (see command `WAVELENGTH`) used for input of the peak positions.

`DEL_2THETA` will typically be in the range 0.05 to 0.20 for most searches. For materials where the lattice dimensions may vary (i.e. solid solutions), or where either the observed peaks or the database are presumed inaccurate, larger values may be needed.

`/R_INDEX=Req_Index`
`/Rmin=R_Imin`

Req_Index and R_Imin determine how the "Required Lines" screening step in the REDUCE command is performed. In this step, entries from the the starting subfile (see command STARTFILE) are dropped from consideration unless one of the observed peaks matches a peak from a peak index. This screening step may be skipped, if desired, by setting Req_Index to a value of 100 or greater.

Each non-excluded peak in the observed pattern with intensity above R_Imin% of the strongest non-excluded observed peak will be checked in this step to see if matches within DEL_2THETA of a peak in the peak index selected by Req_Index. Thus, this step will reject from further consideration as a potential match patterns that do not have at least one observed peak matching some peak in the JCPDS-ICDD database.

The allowed values for R_Imin are between 0 and 99. The allowed values for Req_Index are between -1 and 100 and have the following meaning:

- `100` Skip the "Required Line" step.
- `-1` Use the "Three Strongest" Peak Index file.
- `n` Use the "n% and Above" Peak Index file (n = 0 to 99). Note that if the requested index file is not available, the next smallest file (at 10% increments) will be used.

R_Imin will typically be a fairly small number, 5-10%. For patterns with many peaks, where the REDUCE step does not eliminate many entries from consideration, it may be desirable to raise R_Imin up to the range of 25% or higher.

Req_Index will typically be 70% or -1 ("Three Strongest") so that only patterns with reasonably strong matching peaks will be located. If there is fairly strong preferred orientation or other errors which increase the likelyhood that strong peaks will not match between patterns, it may be necessary to use a lower value, 30% or 0%, for Req_Index.

Likewise, when the range of excluded regions in the search becomes large, the probability that the excluded regions will contain all of the strong peaks in the desired matching phase and thus the pattern will not be found. The likely situations where this may occur is when data were collected only over a small region of 2θor when looking for a minor phase, where a large number of peaks in the pattern have already been identified. In these circumstances, if finding appropriate matches becomes difficult, lower Req_Index or even turn off this step (by setting Req_Index to 100).

`/F_INDEX=Forbid_Index`
`/FWidth=FWHM`
`/Fmin=F_Imin`

Forbid_Index and F_Imin determine how the "Forbidden Lines" screening step in the REDUCE command is performed. In this step, entries from the the starting subfile (see command STARTFILE) are dropped from consideration if there is a peak in a peak index that falls in an area of the pattern where no peaks greater than F_Imin% are observed.

In this step, the pattern is broken up into approximately 260 regions. Each region is checked to ensure that there are no peaks greater than F_Imin% of the strongest non-excluded observed peak within FWHM degrees and that the region has not been marked as excluded. If there are no peaks and no excluded regions, the peak index selected by Forbid_Index is checked for peaks in this region. Any peak found in the region will eliminate the entry from further consideration.

The pattern is processed using using peak positions transformed to angles for Cu Kα_1 radiation. Thus, FWHM defines a width in units of degrees 2θ for Cu Kα_1 radiation, regardless of the wavelength mode (see command WAVELENGTH) used for input of the peak positions.

The allowed values for F_Imin are between 0 and 99. The allowed values for Forbid_Index are between -1 and 100 and have the following meaning:

100 Skip the "Forbidden Line" step.

-1 Use the "Three Strongest" Peak Index file.

n Use the "n% and Above" Peak Index file (n = 0 to 99). Note that if the requested index file is not available, the next smallest file (at 10% increments) will be used.

F_Imin will usually be a fairly small number, 1-4%, and Forbid_Index will typically be in the range of 30-50%. This implies that a JCPDS-ICDD peak in the range of 30-50% will be observed in the experimental pattern at least at the 4% range. This may not be true if the specimen has extreme preferred orientation or is composed of several phases where no phase constitutes a majority of the sample or if the JCPDS-ICDD pattern has preferred orientation. In these cases, where the REDUCE step leaves no reasonable materials as potential "hits", one should lower F_Imin, perhaps as low as 0% and/or raise Forbid_Index to 70-90% or -1. In extreme cases, for example, where one want to find matches to JCPDS-ICDD patterns where stong peaks may be completely missing from the observed pattern, it may be necessary to skip this step (by setting Forbid_Index to 100.) For materials where the REDUCE step does not eliminate enough entries from consideration, it may be desirable to raise F_Imin up to the range of 10-15% and set Forbid_Index to 30%.

/MAXDBMISS=DB_max_miss
/DB_IMIN=DB_min_int

In the MATCH step, the JCPDS-ICDD entries are compared one at at time to the observed peaks. The number of peaks in the JCPDS-ICDD pattern that must be matched for the entry to be given further consideration is dictated by the values of DB_max_miss and DB_min_int. All JCPDS-ICDD entries that do not match this criteron are removed from the list of possible "hits."

For a pattern to be considered a likely match for an entry one expects most if not all of the strong peaks in the JCPDS-ICDD entry to be observed. Weak peaks may not always be seen depending on the relative amount of the phase and the quality of the sample and the pattern. A pattern will be discarded if more than DB_max_miss peaks above DB_min_int% relative intensity are not within DEL_2THETA of an observed peak. Thus DB_min_int% determines the threshold for what is considered to be an observable intensity level. If the material is believed to be single phase, DB_min_int should be a fairly larger number, 10-20%. But for identifying phases in a material with many phases, it may be necessary to raise

DB_min_int as high as 50%. Under circumstances, the observed peaks should match all of the JCPDS-ICDD peaks and DB_max_miss should be 0 or at most 1. However, any of the following conditions can lead to strong JCPDS-ICDD peaks to be missing from an observed pattern: severe preferred orientation in the observed (or database!) pattern; an impurity in the database pattern (rare but sometimes occurs); peak shifts due to instrumental errors.

In general it makes sense to start with small values for both DB_max_miss and DB_min_int. If no appropriate "hits" are found. It is advisible to raise first DB_min_int and then DB_max_miss. Both values must be integers.

/MATCHOBS=OBS_min_lines
/OBS_IMIN=OBS_min_int

In the MATCH step, the JCPDS-ICDD entries are compared one at at time to the observed peaks and patterns that do not match the observed pattern are removed from further consideration. Entries are removed unless at least OBS_min_lines percent of the lines above OBS_min_int percent relative intensity are matched.

In general it makes sense to start with values in the range of 50% for OBS_min_lines and 25% for OBS_min_int. Meaning that a database entry must match at least half of the observed lines above 25% relative intensity. If the MATCH step fails to find any likely "hits," it is wise to lower OBS_min_lines and/or raise OBS_min_int so that fewer lines need to be matched for a hit to be obtained. Lower OBS_min_lines first, if a multiphase mixture is suspected.

If too many "hits" are found to review conveniently, it is wise to increase OBS_min_lines and/or lower OBS_min_int. If a multiphase mixture is suspected, lower OBS_min_lines first.

/MAXCARDS=MAX_hits

The MATCH step will be ended early if more than MAX_hits entries are found in the search. This can be used to prevent "run-away" searches which turn up too many entries to comfortably review. When the search is performed interactively, the search can either be continued or abandoned if the MAX_hits threshold is reached.

The default value for MAX_hits is 999. If this many entries are located, it is likely that the criteria for the REDUCE and MATCH are too broad and the run will need to be repeated. For very slow computer systems or where CPU time is at a premium, it may be wise to lower this value. Under most conditions the value of MAX_hits is unimportant.

/SORT=Num_Sort
/SORT
/NOSORT

This controls sorting of entries by figure of merit (FOM) in the REPORT (or SEARCH) command. If Num_Sort is positive, the step will list the Num_Sort ICDD-JCPDS entries with the best FOM and a subfile with these entries will be written. If Num_Sort is zero or /SORT is specified without a number for Num_Sort the sort will be performed but all "hits" from the MATCH (or REDUCE step, if MATCH is skipped) will be listed in the report. Using a negative value for Num_Sort or specifying /NOSORT prevents sorting, speeding the REPORT step.

`/FOM=Calc_type`

Determines how the overall figure of merit (FOM) is computed in the Report command.

If `Calc_type` is 1, differences between matching observed and ICDD-JCPDS peak positions do not affect the overall FOM.

If `Calc_type` is 2, differences between observed and ICDD-JCPDS peak intensities do not affect the overall FOM.

If `Calc_type` is 3, the full-pattern FOM formula is used for the overall FOM. This option is appropriate only if a raw data file has been input to the program and also requires that the background be subtracted from the data before it is read into the program.

See the previous section on the `REPORT` command for more details on the computation of figures of merit.

`/NAME=search_name`

This qualifier is used to to define the names that will be used for files that will be created during the run. While this name may be as long as 40 or more characters (VMS allows very long filenames), for convenience, the name will typically be 4 to 10 characters. The search name is subject to the normal VMS conventions governing file names: all letters, numbers and some symbols (notably `_` and -) are allowed, but spaces and most other symbols are not allowed.

If files are to be written in a directory or disk other than the current default, device specifications may be included in the `search_name`. File extensions are allowed, but their use is not recommended. If supplied, the file extension will be used for naming the "load file" only.

The following files are created by program SEARCH:

> The "load file" is used for temporary storage of the current SEARCH settings. This file may be reread by a later run of SEARCH and will also be used if SEARCH is run as a batch job. The file name is taken from the search name. File extension `.SEA_IN` is used, if none is specified in the search name.
>
> The "starting subfile" is created if the `STARTFILE` command is used to narrow down the number of entries to be considered during the search by creating a user supplied subfile. The file is written by program LOGIC. The subfile to be written will be named using the current search name, however, the device/directory will be changed to the scratch directory, `PS_TMP`, the string "`_SEARCH`" will be appended to the search name, and the file extension will be set as `.USRPDF`.
>
> The "search output file"is a user subfile with the matches (hits) from the search. This file may be read by program LOGIC. The file will be named directly from the search name; the file extension will be `.USRPDF`.
>
> The "top hits output file"is a user subfile with the best ranked matches from the `SEARCH` or `REPORT` command if sorting has been requested. The file is the same as "search output file" except `_TOPxx` is appended

to the search name (`xx` is the number of sorted entries).

3.17 Command SHOW

This command is used to display the parameters which govern the search, as established by command `SET`.

3.18 Command STARTFILE

This command is used to select the entries in the ICDD-JCPDS database that will be considered when performing the search. The entire database may be searched or the search may be restricted to a smaller section (subfile). A number of standard subfiles have been prepared by the ICDD-JCPDS; alternately program LOGIC may be used to prepare a user-defined subfile.

Use of a subfile (any option other than `/SUBPDF=FULL`) reduces the number of entries that need be examined, which can greatly speed the search. For example, if it can be assumed that no elements heavier than iodine are present in the unknown, program LOGIC can be used to eliminate approximately one-third of the entries in the database from consideration. (This is performed using command

```
CULL/E_SP=(Xe,Lr)/OR
```

within program LOGIC.)

Program LOGIC is most commonly used to specify chemistry constraints. To call program LOGIC from within SEARCH, enter command `STARTFILE/LOGIC`. To read a subfile previously prepared by LOGIC and stored in a user-defined file, use command `STARTFILE/USERFILE=file_name` to select that file. The user-defined subfiles created at the end of SEARCH run may also be used as a starting point.

Only one of the following three options may be specified.

QUALIFIERS

`/LOGIC` — Specify this qualifier to call program LOGIC to create a new user-supplied subfile to be used in the search. When the LOGIC program is exited, a subfile will automatically be written and program SEARCH will be resumed. The subfile to be written will be named using the current search name, however, the device/directory will be changed to the scratch directory, `PS_TMP`, the string "`_SEARCH`" will be appended to the search name, and the file extension will be set as `.USRPDF`.

`/USERPDF=file_name` — Use a previously written user-supplied subfile with name `file_name`. The default file extension is `.USRPDF`.

`/SUBPDF=sub_file` Use this option to start from one of the standard subfiles, such as the the inorganic subfile.

The available subfiles are:

FULL	all entries in the database
NULL	null table (a table without any entries)
INORGANICS	Inorganic materials
ORGANICS	Materials with a C-H bond
COMMON	commonly found materials or phases
MINERALS	Minerals, natural and synthetic
METALS	metals, alloys and related materials
NIST	patterns recorded by NIST (NBS)
FORENSIC	materials of forensic interest
ZEOLITES	zeolites and molecular sieves
DELETED	superceeded but not removed patterns (if any)
LOCAL	locally defined patterns (if any)
SUPERCON	superconductors and related materials
EXPLOSIVES	explosives and related materials
EDUCATION	educationally relevant materials
CEMENT	materials related to cement production
CORROSION	corrosion products and related materials Only one subfile may be specified. To search two subfiles, (for example the MINERALS and METALS subfiles) use program LOGIC (see `/LOGIC`) to `OR` (`ADD`) together these two subfiles.

Note that the `sub_file` name may be abbreviated by only including the initial letters as long as the name is uniquely specified. Also note that "DELETED" patterns are not used unless the `DELETED/INCLUDE` command is used to force inclusion of these patterns.

3.19 Command TITLE

Used to change the "search title." The only purpose of the search title is to provide a mechanism for saving comments and other information from a search in the "load file."

The format of this command is:

```
TITLE title
```

The title can be specified on the command line or will be prompted. If the title is put on the command line, any lower case letters used in the title will be converted to uppercase.

EXAMPLES

`TITLE This is the new title for the search`	Note that the title will be converted to all capital letters.
`TITLE`	The user will be prompted to specify a title.

3.20 Command WAVELENGTH

Peaks positions may be input or output as d-spacings (in Å) or as 2θ (Bragg) angles corresponding to a given x-ray or neutron wavelength. This command is used to select between d-spacings and angles and to select a wavelength for the latter option.

The current mode of the program is displayed in the header line at the top of the computer screen. The default when the program is started is determined by logical name `PS_WAVELENGTH`. If this logical name is not defined, the default is to operate in d-space mode. When the `WAVELENGTH` command is used logical name `PS_WAVELENGTH` is redefined and this becomes the new default mode.

PARAMETER

`wave_length` — A single wavelength value may be specified directly, where `wave_length` is the x-ray or neutron wavelength in Å. (The `target_type` will be assumed to be `SY` for synchrotron radiation).

If `0.0` is used for the `wave_length`, the program will enter d-space mode (equivalent to specifying (`WAVELENGTH/NOTARGET`).

If `wave_length` is used, `/TARGET` and `/WTYPE` should not.

QUALIFIERS

`/TARGET=target_type`
`/TARGET`
`/NOTARGET`

Specifies an x-ray target for conventional x-ray sources. The choices for targets are: `Cu`, `Mo`, `Ni`, `Co`, `Fe`, `Cr`, `Ag`, `NU`, or `SY`. Specifying `/TARGET` without a `target_type` is equivalent to `/TARGET=CU`. (Capitalization of the target type is ignored.)

If `NU` or `SY` (for neutron or synchrotron radiation) is used, the program prompts for a wavelength.

For input/output using d-spacings specify `/NOTARGET`

The `/TARGET` option cannot be specified with a `wave_length` value.

`/WTYPE=wave_type` `wave_type` may be either 1, 2 or 3 which determines the exact value used for the wavelength specified with `/TARGET`. The choices are:

1 to use Kα_1 radiation

2 to use Kα_2 radiation

3 to use the intensity weighted average of Kα_1 and Kα_2 radiation.

Specifying `/WTYPE` without a value for `wave_type` is equivalent to specifying `/WTYPE=1`.

This qualifier is ignored if the radiation source has a single wavelength, (e.g. `/TARGET=NU` or `/TARGET=SY`) or a `wave_length` is specified.

EXAMPLES

`WAVELENGTH/TARGET=CU/WTYPE=3`
The wavelength will be set to the average of Cu Kα_1 and Kα_2.

`WAVELENGTH/TARGET` The wavelength will be set to Cu Kα_1.

`WAVE/NOTAR` Peaks positions, etc. will be displayed as d-spaces.

`WAVE 0.0` Peaks positions, etc. will be displayed as d-spaces.

`WAVE 2.5401` The wavelength will be set to 2.5401Å.

`WAVE` The user will be prompted to choose a wavelength or two use d-spacings.

`WAVELENGTH/TARGET=NU/WTYPE=3`
The user will be prompted to enter a wavelength; the `/WTYPE=3` qualifier will be ignored.

Chapter 4: Program CMPR

Program CMPR is used to perform operations that compare diffractograms: operations such as plotting, addition/subtraction and simulation of patterns from ICDD-JCPDS data.

4.1 Command ADD

Used to add two files. The file numbers can be entered on the command line or can prompted. File numbers may be separated by either spaces or commas (or both).

`ADD 2 4` is equivalent to `ADD 2,4`

QUALIFIERS

`/TITLE="file_title"` This option is used to specify a title line for the new file

`/SCALE=scale_factor` The intensities in second file will be multiplied by `scale_factor`. The `scale_factor` need not be an integer, but should be greater than zero.

`/OFFSET=offset_val` A fixed offset can be added (`offset_val` greater than zero) or subtracted (`offset_val` less than zero) to the resultant diffractogram after the two files are added. `offset_val` will be added to each point; `offset_val` may be a floating point number.

If `/MINIMUM` is used with `/OFFSET`, the offset, `offset_val`, is added after subtracting the minimum intensity from all points, thus if the command `SUB/MIN/OFF=100` is used, the lowest intensity point in the pattern will have an intensity of 100.

`/MINIMUM` Subtracts the intensity of the least intense point from all points in the diffractogram.

4.2 Command ATTRIBUTES

This command is used to set the attributes which define how a diffractogram is plotted. The files to be affected may be included on the command line or may be input with a prompt. If more than one file is specified, the attributes for all specified files will be set to the same values.

QUALIFIERS

`/COLOR=color` Sets the color for plotting the diffractogram. The color index must be a number between 0 and 255, where color 0 corresponds to the background color (producing an invisible plot). The actual number of colors available isdetermined by the graphics device (see the PGPLOT documentation) with most devices supporting less than 256.

`/WIDTH=width` The line width to be used for plotting the diffractogram and/or the peak positions. A width of 1 is the usual default, but thicker lines may be specified by using larger numbers. Numbers less than 1 should not be used.

`/LINE=line_type` Determines the type of line used for plotting the diffractogram intensity versus angle data. `line_type` of 1 produces a single connecting line. `/LINE=2` through `/LINE=5` produce dashed, dot-dashed, dotted and dot-dot-dashed lines, respectively. `/LINE=6` puts dots at each data point (this is not exactly the same as a dotted line.) A line type of 0 indicates that the diffractogram data is not to be plotted. Numbers less than 0 or greater than 6 should not be used.

`/PEAK=peak_type` Determines the type of line used for plotting the peak position data. Ignored for files that do not have peaks. A `peak_type` of 1 produces a single straight line for each peak. Types of 2 through 5 produce dashed, dot-dashed, dotted and dot-dot-dashed lines, respectively. A peak type of 0 indicates that the peaks are not to be plotted. If 8 is added to the peak type, the intensity is considered arbitrary and will be plotted full scale. Numbers less than 0 or greater than 14 should not be used.

`/OFFSET=off_value` Specifies an offset to be added to the data when the data is plotted. The value is a floating point number which may be positive or negative.

`/MAGNIFICATION=mag_value`
Specifies a magnification factor for the data for plotting. The value is a floating point number which may be greater than or less than one.

`/ALL` Sets the specified attributes for all files.

EXAMPLES

`ATT 1 2 3` Sets the attributes for files 1, 2 and 3. The values for the attributes will be requested using prompted input.

`ATT` As before except the file numbers will also be prompted for.

`ATTR/COLOR=2 4,3` Resets the color for files 3 and 4 to color type #2 (actual color is device dependant, usually red).

`ATTR/ALL/C=1` Resets the color for all files the default color.

4.3 Command COMBINE

Used to combine two or more files into one file. The file numbers can be entered on the command line or can be prompted. File numbers may be separated by spaces or commas or both.

Command format: `COMBINE [file_list]`

PARAMETER

`file_list` File numbers may be specified on the command line separated by commas or spaces.

If no files are placed on the command line, a prompt will be generated for file numbers.

4.4 Command DCL

Spawns a subprocess to execute DCL commands, type LOGOUT to return back to CMPR without affecting the current list of files. This command is useful for quick DCL "errands" such as answering a mail message without exiting the program.

4.5 Command DEFAULT

This program can operate in two modes, AUTO mode and MANUAL mode. In AUTO mode, default values are used where possible to cut down on the amount of questions the need to answered. In MANUAL mode, if a parameter is not specified on the command line, a prompt will be generated for an option or value. The current mode is listed on the top of the screen.

Command qualifiers always override default options. For example, in AUTO mode command `WRITE/NBS` produces a file in NBS format, while `WRITE` defaults to `/BINARY`. In MANUAL mode, the latter command would generate a prompt requesting a choice for file format.

The mode can be toggled by entering the DEFAULT command without any qualifiers. Alternately, a qualifier may be used:

`DEF/MAN` (sets the mode to MANUAL)

`DEFAULT/A` (sets the mode to AUTO)

`DEF` (sets the mode to the opposite of the current mode)

QUALIFIERS

`/AUTO`
`/NOMANUAL` If either of these qualifiers are used, the mode is set to AUTO. Thus, default values will be used for options (where possible) to reduce the number of prompts. (`/NOMANUAL` is equivalent to `/AUTO`)

`/MANUAL`
`/NOAUTO` If either of these qualifiers are used, the mode is set to MANUAL. Thus, the program will prompt rather than using default option(s). (`/MANUAL` is equivalent to `/NOAUTO`)

4.6 Command DELETE

Used to remove a "file" from the list of available files. This will not delete the file from disk storage (unless it was created in CMPR and never actually written on disk). Only one file can be removed at a time and file number 1 can only be removed with the `DELETE/ALL` command – which removes all files (equivalent to starting a new CMPR run).

usage:

`DELETE [file_number]` or

`DEL/ALL`

PARAMETER

`file_number`	The number of a single file to be removed may be specified on the command line. If the file number is not specified a prompt will be given requesting a file number. The file number must be in the range of 2 to 10. No file number may be specified if `/ALL` is used.

QUALIFIER

`/ALL`	Removes all files (equivalent to starting a new session). When running interactively, a prompt will be generated for new file names to read. No file numbers can be specified if `/ALL` is specified.

4.7 Command DGEN

Computes the allowed d-spaces for a given unit cell optionally omitting reflections extinct by translation symmetry. Must be run interactively.

QUALIFIER

`/A=a_length`
`/B=b_length`
`/C=c_length`
`/ALPHA=bc_angle`
`/BETA=ac_angle`
`/GAMMA=ab_angle`
	Defines the unit cell lengths in Angstroms and the angles in degrees for the d-space generation. If `a_length` is not specified, values for the cell Laue symmetry and then all appropriate unit cell parameters will be requested. If `b_length` and/or `c_length` are not specified, they default to `a_length`. Any angles that are not specified default to 90 degrees.

4.8 Command EXIT

Type EXIT (which can be abbreviated to E) to exit; alternately press Control Z (`^Z`) to exit the program. After exiting, you will be prompted to write any files that have been modified or created within the program.

4.9 Command FILE

Allows a series of commands to be input to the program from an external file. The file should be prepared before starting the program, or using the DCL command to invoke an editor.

PARAMETER

`file_name` A single file may be specified on the command line containing the name of the file with commands. If the file is not specified, a prompt will be given to request a file name.

If no file extension is supplied, the default extension is `.CMD`

4.10 Command HKLPLOT

Used to label hkl values and show which peaks would be expected to become extinct for a given set of symmetry elements.

A symmetry operation is supplied to the program and reflections from the file are displayed in one of three colors (or line styles if the graphics device is incapable of displaying color graphics). The basic color is used for peaks that are extinct by the specified Bravais lattice and translational symmetry elements. The second color is used for peaks that are not extinct. A third color is used for where extinct and non-extinct peaks overlap.

If raw data is in the diffractogram file, that data is also displayed. If two file numbers are given, the data from the second file is displayed.

If the interactive graphics device has a graphics cursor, the cursor can be used to selectively label the indices of selected reflections.

QUALIFIER

`/WIDTH=P_width` The value of `P_width` dictates the width where it is expected to be impossible to discern two overlapped reflections. This should normally be in the range of one and a half to one quarter of the expected peak FWHM.

`/XLOW=low_limit`
`/XHIGH=high_limit` Defines the limits for plotting the x-axis. If either is specified, the values for limits will not be prompted. Values may be integers or floating point numbers, but must be included if the qualifier is specified. The units are degrees 2θ.

`/DATASCALE=data_scale`
`/PEAKSCALE=peak_scale` Defines the limits for plotting the y-axis. A value of `1.0` means data/peaksare plotted so that the maximum value is full scale, `2.0` means a magnification factor of x2.

A value of `0.0` for `peak_scale` means that all peaks will be plotted to full scale.

4.11 Command LOGIC

Use this command to invoke the LOGIC program to search the ICDD-JCPDS database (without exiting CMPR.) After exiting from LOGIC, CMPR will be resumed with all current files still loaded and all current parameters unchanged.

4.12 Command MANIP

Use this command to invoke the MANIP program without exiting CMPR. When exiting from MANIP, the computer will return to CMPR with all CMPR files still loaded in memory. It is possible to pass a file from CMPR's list of current files to MANIP and/or pass one or more files from MANIP back to CMPR.

PARAMETER

`file_number` The number of a single file may be specified on the command line referencing the number of the file to be passed to MANIP. If the file number is not specified a prompt will be given requesting a file number. Files must be written on disk in order to be passed. If the file has been modified and does not exist in the current form on disk, confirmation will be requested before the file is written.

4.13 Command PLOT

Used to produce a plot on either a terminal or on a hard copy device. Several options are available to determine the format of the plot.

The default options for plotting are determined by the DEFAULT command. However, use of a PLOT qualifier on the command line will override the default option.

Note that the x-axes for all files to be plotted should be of the same x-axis type (have the same units) except if `/Q`, `/WAVELENGTH` or `/DSPACE` is specified. In that case files will be converted (if possible) to the appropriate units before plotting.

Command format: `PLOT [/qualifiers] [file_list]`

PARAMETER

`file_list` File numbers may be specified on the command line separated by commas or spaces:

```
PLOT 1,2,3
PLOT 1 2 3
PLOT 1 2,3
```

all of the above are equivalent and valid.

If no files are placed on the command line, a prompt will be generated for file numbers.

QUALIFIERS

`/XLOW=low_limit`
`/XHIGH=high_limit`

Defines the plot limits for the x-axis. If either is specified, the values for plotting limits will not be prompted. Values may be integers or floating point numbers, but must be included if the qualifier is specified. The units are those of the files to be plotted unless the the `/Q`, `/WAVELENGTH` or `/DSPACE` option is used.

`/Q`
`/DSPACE`
`/WAVELENGTH=wavel`

Files are plotted with their x-axis units unchanged unless `/Q`, `/DSPACE`, or `/WAVELENGTH` is placed on the command line or the default plotting option is changed to one of these options. The program will then attempt to convert all files to the requested units (not all conversions are possible.)

`/Q`

The graph will be plotted in Q units (in reciprocal Å). Q is defined as

$$Q = \frac{4\pi}{\lambda}\sin\theta = \frac{2\pi}{d}.$$

`/DSPACE`

The graph will be plotted in D-space units (in Å). the d-space is defined as

$$d = \frac{\sin\theta}{2\lambda}.$$

`/WAVELENGTH`

The graph will be plotted in 2θ units at wavelength `wavel`Å.

`/STACK`
`/NOSTACK`

There are two options that govern how more than one diffractogram is plotted. They may be superimposed on a single set of axes, with optional offsets between plots (see `/XSTACK` and `/YSTACK`) or plotted with each diffractogram having a separate set of axes. These options are only applicable if more than one file will be plotted.

`/STACK`

Causes each diffractogram to be plotted with single set of axes. These plots are also called single-box plots in the documentation.

`/NOSTACK`

Causes each diffractogram to be plotted with a separate set of axes. These plots are also called multiple box plots in the documentation.

`/XSTACK=X_spacing`
`/YSTACK=Y_spacing`

Causes plots to be "stacked" – drawn on a single set of axes (see `/STACK`). `X_spacing` is the horizontal distance in percent of the full scale and `Y_spacing` is the vertical distance in percent of full scale between the zero values in successive plots. `/XSTACK` and/or `/YSTACK` cannot be used with the `/NOSTACK` qualifier.

`/RELATIVE`
`/EXTREME`
`/FIRST`

There are four scaling options to determine the maximum value for the y-axis. The first three are applicable only if more than one file will be plotted.

`/FIRST`

> The maximum intensity for the vertical axis is set from the first file to be plotted.

`/EXTREME`

> The maximum intensity for the vertical axis is set from the maximum of all files to be plotted. All files will be plotted on the same scale.

`/RELATIVE`

> The vertical axis is set to the maximum point in each diffractogram. If the plot is "stacked" (see `/XSTACK` or `/YSTACK`) the full scale will be increased, if needed to include all files.

The fourth option is to specify the maximum [and optionally minimum] y-axis values using `/YHIGH` [and `/YLOW`.]

Only one of `/YHIGH`, `/EXTREME`, `/FIRST` and `/RELATIVE` can be used.

`/YLOW=low_limit`
`/YHIGH=high_limit`

Defines plot limits for the y-axis. `low_limit` and `high_limit` are the minimum and maximum number of counts that can fit on the plot axes. (These numbers need not be integers and are not prompted.) If `/YLOW` is not specified, `low_limit` will be 0. If `/YHIGH` is not specified, `high_limit` will depend on options for `/XSTACK` or `/YSTACK`.

Cannot be used with `/EXTREME`, `/FIRST` or `/RELATIVE`.

`/SIZE=(X_len,Y_len,X_mar,Y_mar)`
`/SIZE=(X_len,Y_len)`
`/SIZE`

Used to specify the size of the plot in inches. `X_len` and `Y_len` are the lengths of the x- and y-axes, respectively. `Y_mar` and `X_mar` are the margins below and to the left of the axes. (The default margins are 1 inch.) These numbers may be floating point numbers.

The command can be used two ways, if `/SIZE` is used without any values, CMPR will prompt for values. If values are specified on the command line, both `X_len` and `Y_len` must be specified. `X_mar` and `Y_mar` are optional, but `X_mar` must be specified before `Y_mar`.

It is the user's responsibility to insure that the requested size is compatible with the graphics device.

`/TITLE`
`/NOTITLE`

If `/TITLE` is specified, plot(s) will be labeled with the title from each file. If `/NOTITLE` is specified, plot(s) will not be labeled with the title.

(Command `TITLE` may be used to change the file title).

`/FILE`
`/NOFILE`

If `/FILE` is specified, plot(s) will be labeled with the name of the data file. IF `/NOFILE` is specified, plots will not be labeled with the filename.

`/CLIP`

Segments of the plot that lie outside the plot axes may "squared off" (clipped) at the axis limit (`/CLIP`) or may be simply omitted (`/NOCLIP`).

`/LINEAR`
`/LOG`
`/SQRT`
	The intensity scale can plotted proportional to the number of counts (`/LINEAR`), logarithmic units (`/LOG`) or proportional to the square-root of the number of counts (`/SQRT`). Plots will be made in `/LINEAR` mode, unless `/LOG` or `/SQRT` is specified or the default is changed.

`/GRID`	If `/GRID` is specified, the graph will be plotted with a grid extending from each tick mark on the x- and y-axes.
`/HARD`	If `/HARD` is specified, graphics will be sent to the default hardcopy device, rather than displayed the terminal.

4.14 Command QUIT

Type QUIT (which can be abbreviated to Q) to quit the program. Unlike the exit command, you will not be prompted to write any files that have been modified or created within the program.

4.15 Command READ

Used to read one or more new files into the list of available file names. (Assuming there is still space in the list for additional files. If not, first use the DELETE command to make room.)

usage: `READ [filename1] [,filename2] [,filename3],...`

See the section on File Formats in the first chapter for information on formats for peak and data files.

PARAMETER

`file_name`
`file_name_1, file_name_2,... file_name_8`

Files may be specified on the command line. If no files are specified, a prompt will be given requesting a file name to read.

`file_name` may be VMS filename or logical name or a JCPDS-ICDD entry number. For interactive input, a question mark (`?`)may be used to see help information and if a wildcard is used (`*` or `%`), a directory listing is shown.

If `file_name` is a VMS filename it can be of form `FILE.EXT` or `DEV:[DIR]FILE.EXTENSION;2` – subject to a limitation that the file name must not exceed 80 characters.

It is usually preferable to supply the file name without a file extension, as the default extension will then depend on the file format. This improves the speed that the program has available when searching for the file. The subroutines which read data and peak files, (subroutines `READDATA` and `READPEAK` respectively), will attempt to determine the format of the file from the file contents and the extension.

More than one file name can be specified on the command line, but names must be separated by commas. If more file names are specified than may be read, the extra names will be ignored.

Filenames may not be specified if the `/JCPDS` qualifier is used.

QUALIFIER

`/FORMAT=fileform` This optional qualifier may be used to specify the file format that will be used for reading the file(s). If more than one file is given and `/FORMAT` is used, all files must all be in the specified format. (See the information on File Formats for the `fileform` codes).

In most cases it is not necessary to specify the file format, as the program will discern the file format from the file. However, in certain cases where problems are encountered, it may be necessary to use the format option.

File formats may not be specified if the `/JCPDS` qualifier is used.

`/JCPDS=card_list`
`/JCPDS` Use this qualifier to select entries using their ICDD-JCPDS entry number. The entry number is always a five or six digit number consisting of the "old" entry number plus 10,000 times the set number. For example, entry 413 in set 7 would be coded as:

EXAMPLES

```
READ group.mother/FORMAT=DUPONT
```

```
READ
READ/JCPDS=(271402,400001)
```

```
READ group.mom,[.test]exper.fil,somewhere:overthe.rainbow;1
```

4.16 Command SCALE

Rescales the x and/or y values for a data file.

PARAMETER

`file_number` The number of a single file to be rescaled may be specified on the command line. If the file number is not specified a prompt will be given requesting a file number.

QUALIFIERS

`/YMULT=Y_Factor`
`/YOFFSET=Y_Offset`
: Rescales the y-values in the file from by first adding the offset (`Y_Offset`) and then by multiplying the y-values by the multiplier (`Y_Factor`).

If not specified, `Y_Offset` defaults to 0.0 and `Y_Factor` defaults to 1.0. If neither value is specified, a prompts will be generated for values. /XMULT=X_Factor

/XOFFSET=X_Offset

Rescales the x-values in the file from by first adding the offset (`X_Offset`) and then by multiplying the x-values by the multiplier (`X_Factor`).

If not specified, `X_Offset` defaults to 0.0 and `X_Factor` defaults to 1.0. If neither value is specified, a prompts will be generated for values.

4.17 Command SIMULATE

This option is used to construct a simulated diffraction pattern from a set of peak positions and intensities. The peak positions may be generated by an external program, such as Lazy/Pulverix, read from the JCPDS-ICDD data base, or obtained from an experimental source.

The peak positions must be loaded into one or more files using the `READ` command. This command may then be used to construct a simulated pattern by convoluting that data. More than one set of peaks may be combined to simulate a mixture, in which case weights for each file may be specified.

If one or more files will be combined, or the file to be convoluted already has a corresponding diffraction pattern, a new file will be created. If only one file is used and no diffractogram is present for that file, the diffractogram will be added to the same file as the peaks

The command format is:

```
SIM [file_1] [file_2]... [file_8] [/qualifiers]
```

PARAMETER

`file_list`
: File numbers may be specified on the command line separated by commas or spaces.

If no files are placed on the command line, a prompt will be generated for file numbers.

QUALIFIERS

`/RANGE=(x_min,x_max)`
`/RANGE`
: Specifies the 2θ range of the simulated pattern. If only `x_min` is specified, `x_max` defaults to the largest x value in file #1. If both numbers are omitted, both default to the same as file #1. The numbers may be specified as floating point.

`/WEIGHT=(Wt_2,Wt_1,...Wt_n)`
: Specifies the weights for the `n` files to be convoluted. The default value is 100.

`/STEP=step_size`
`/STEP`
: Specifies the 2θ step size for the simulated pattern in units of degrees. If the value is omitted, the default is the same as the step size in file number #1. `step_size` should always be less than 1.0 but greater than 0.

`/CAUCHY=(p_wid,p_ang)`
`/CAUCHY`
`/GAUSSIAN=(p_wid,p_ang)`
`/GAUSSIAN`
: Selects the peak profile as either Lorentzian (Cauchy) or Gaussian (not both). If both `p_wid` and `p_ang` and are specified, peaks at angle `p_ang` will have a WIDTH of `p_wid` degrees. If both numbers are not specified, the NBS width table will be used. Either number may be floating point.

`/OFFSET=offset_val`
: A fixed integer offset of `offset_val` counts can be added to the simulated pattern. Cannot be used with `/AMORPHOUS`.

`/AMORPHOUS=(a_wid,a_ang,a_int)`
: Specifies that a broad peak simulating amorphous scattering be added to the simulated pattern. A peak will be placed at angle `a_ang`, with width `a_wid` and intensity `a_int`. The default values for `a_ang`, and `a_wid` are 25 and 30 degrees 2θrespectively, for `a_int` it is 2 percent of full scale. Any of these numbers may be floating point values.

  Cannot be used with `/OFFSET`.

`/WAVELENGTH=wave_length`
: A single wavelength may be specified, where `wave_length` is the x-ray or neutron wavelength in Å. If `wave_length` is used, `/TARGET` and `/WTYPE` should not. (The `target_type` will be assumed to be `SY` for synchrotron radiation).

`/TARGET=target_type`
`/TARGET`
: Specifies an x-ray target for conventional x-ray sources. The choices for targets are: `Cu`, `Mo`, `Ni`, `Co`, `Fe`, `Cr`, `Ag`, `NU`, or `SY`. Specifying `/TARGET` without a `target_type` is equivalent to `/TARGET=CU`. (Capitalization of the target type is ignored.)

  If `NU` or `SY` (for neutron or synchrotron radiation) is used, the program prompts for a wavelength. This option cannot be used if a `wave_length` value is specified using `/WAVELENGTH`.

`/WTYPE=wave_type`
: `wave_type` may be either 1, 2, 3 or 4 which determines the exact value used for the wavelength specified with `/TARGET`. The choices are:

  1 to use $K\alpha_1$ radiation

  2 to use $K\alpha_2$ radiation

  3 to use the intensity weighted average of $K\alpha_1$ and $K\alpha_2$ radiation.

  4 to use both $K\alpha_1$ and $K\alpha_2$ radiation.

  Specifying `/WTYPE` without a value is equivalent to `/WTYPE=4`.

  This qualifier is ignored if the radiation source has a single wavelength, (e.g. `/TARGET=NU` or `/TARGET=SY`) and cannot be used if `/WAVELENGTH` is specified.

`/NOISE=sig_level` `/NOISE`	Used to add random noise to the simulated diffractogram. Noise will be added at a level of `sig_level` standard deviations. `sig_level` may be floating point and defaults to 2.0
`/MAXIMUM=max_count` `/MAXIMUM`	This qualifier is used to set the maximum intensity in the pattern after scaling to `max_count`. The value for `max_count` must be an integer, if not specified it defaults to 5000 counts.

EXAMPLES

```
SIMUL
SIM 7,413
SIM 7,413,50 7,414,50/CAUCHY/TARGET=MO
```

4.18 Command SUBTRACT

Used to subtract two files. The file numbers can be entered on the command line or can prompted. File numbers may be separated by either spaces or commas (or both).

`SUB 2 4` is equivalent to `SUB 2,4`

(file #4 will be subtracted from file #2)

QUALIFIERS

`/TITLE="file_title"`	This option is used to specify a title line for the new file
`/SCALE=scale_factor`	The intensities in second file will be multiplied by `scale_factor`. The `scale_factor` need not be an integer, but should be greater than zero.
`/OFFSET=offset_val`	A fixed offset can be added (`offset_val` greater than zero) or subtracted (`offset_val` less than zero) to the resultant diffractogram after the two files are subtracted. `offset_val` will be added to each point; `offset_val` may be a floating point number. If `/MINIMUM` is used with `/OFFSET`, the offset, `offset_val`, is added after subtracting the minimum intensity from all points, thus if the command `SUB/MIN/OFF=100` is used, the lowest intensity point in the pattern will have an intensity of 100.
`/MINIMUM`	Subtracts the intensity of the least intense point from all points in the diffractogram.
`/IGNORE` `/CLIP`	Action to be taken if negative intensities are present. If `/CLIP` is used, negative intensities are set to zero, if `/IGNORE` is used, they are left unchanged. These options cannot be used if `/MINIMUM` is used (which will prevent negative intensities by shifting the pattern up). If `/OFFSET` and `/CLIP` are both used, `offset_val` will be added after negative points are clipped to zero.

4.19 Command TITLE

Used to change the title of a file. The format of this command is:

```
TITLE [file_number] title
```

The title can be specified on the command line only if preceeded by a file number, but neither must be specified. At this time, any lower case letters used in the title will be converted to uppercase.

EXAMPLES

`TITLE 1 This is the new title for file number 1`
: Note that the title will be converted to all capital letters.

`TITLE 1`
: using this version, the title will be prompted.

`TITLE`
: Prompts will be generated for the file number and the title.

4.20 Command WAVELENGTH

Used to enter a default wavelength for the READ and SIMULATE command.

PARAMETER

`wave_length`
: A single wavelength value may be specified directly, where `wave_length` is the x-ray or neutron wavelength in Å. (The `target_type` will be assumed to be `SY` for synchrotron radiation).

  If `0.0` is used for the `wave_length`, the program will enter d-space mode (same as specifying `WAVELENGTH/NOTARGET`).

  If `wave_length` is used, `/TARGET` and `/WTYPE` should not.

QUALIFIERS

`/TARGET=target_type`
`/TARGET`
`/NOTARGET`
: Specifies an x-ray target for conventional x-ray sources. The choices for targets are: `Cu`, `Mo`, `Ni`, `Co`, `Fe`, `Cr`, `Ag`, `NU`, or `SY`. Specifying `/TARGET` without a `target_type` is equivalent to `/TARGET=CU`. (Capitalization of the target type is ignored.)

  If `NU` or `SY` (for neutron or synchrotron radiation) is used, the program prompts for a wavelength.

  For input/output using d-spacings specify `/NOTARGET`

  The `/TARGET` option cannot be specified with a `wave_length` value.

`/WTYPE=wave_type` — `wave_type` may be either 1, 2 or 3 which determines the exact value used for the wavelength specified with `/TARGET`. The choices are:

1 to use Kα_1 radiation

2 to use Kα_2 radiation

3 to use the intensity weighted average of Kα_1 and Kα_2 radiation.

Specifying `/WTYPE` without a value for `wave_type` is equivalent to specifying `/WTYPE=1`.

This qualifier is ignored if the radiation source has a single wavelength, (e.g. `/TARGET=NU` or `/TARGET=SY`) or a `wave_length` value is specified.

EXAMPLES

`WAVELENGTH/TARGET=CU/WTYPE=3`
The wavelength will be set to the average of Cu Kα_1 and Kα_2.

`WAVELENGTH/TARGET` — The wavelength will be set to Cu Kα_1

`WAVE/NOTAR` — Peaks positions, etc. will be displayed as d-spaces.

`WAVE 0.0` — Peaks positions, etc. will be displayed as d-spaces.

`WAVE 2.5401` — The wavelength will be set to 2.5401Å.

`WAVE` — The user will be prompted to choose a wavelength or two use d-spacings.

`WAVELENGTH/TARGET=NU/WTYPE=3`
The user will be prompted to enter a wavelength; the `/WTYPE=3` qualifier will be ignored.

4.21 Command WRITE

Write one of the "files" in memory (from the table of available files) onto disk.

PARAMETER

`file_number` — The number of a single file may be specified on the command line referencing the number of the file to be written. If the file number is not specified a prompt will be given requesting a file number.

QUALIFIERS

`/FILENAME=file_name` The name to be used for the file. This overrides the name already associated with the file and will replace that name. If /FILENAME is not specified and CMPR is run interactively, a prompt will be generated for the name of the file.

`/BINARY`
`/NBS`
`/PROFPV`
`/GSAS`
`/JONES`
`/PEAKS`

Determines the format of the file to be written. If CMPR is run in MANUAL mode (see command DEFAULT) and none of these options is specified, a prompt will be generated. (In AUTO mode the default is `/BINARY`)

`/BINARY` writes a file in du Pont format

`/PEAKS` Writes an ASCII file with just the peak information.

EXAMPLES

`WRITE 1` This command causes file #1 to be written. The file name and format will be prompted for (in MANUAL mode).

`write 7/BIN/FILE=tmp:copy.bin`
This command causes file #7 to be written as `TMP:COPY.BIN` in binary format.

`WR/NB` This command causes file #1 to be written in "NBS" format. The file number will be prompted for and in MANUAL mode, so will the file name.

Chapter 5: Customization Instructions

This chapter gives instructions for customizing the Powder Suite package. For the package to operate it must know where to find various files, for example, where the JCPDS-ICDD files are located. In addition the package is written to support a wide range of terminals and graphics devices and the program must be instructed what type of devices it will use. This information is stored in VMS logical names beginning with `PS_` (VMS commands `$ DEFINE` and `$ ASSIGN` define logical names, command

```
$ SHOW LOGICAL PS_*
```

will show the definitions. For convenience, the definitions are defined in one file, but users may override these definitions.

The first time the PS command procedure (`PS.COM`) is used, and at any later time if the INIT option is used, the DCL procedure defines all of the symbols and logical names required by the package which are found in file `PS_EXE:PS_INIT.COM`. This file is located in the same directory as the executable versions of the programs, `[PS.EXE]` or `[dir.PS.EXE]`. When Powder Suite is installed, this file is updated to reflect the definitions need for the local computer environment (device names etc.).

In addition each user can have one or more customized `PS_LOCALINIT.COM` files. When the initialization is done (the first time `PS.COM` is called or when using the menu INIT option), after executing the commands in file `PS_EXE:PS_INIT.COM`, the following locations are searched (in the order specified):

(1) file `PS_LOCALINIT.COM` in the current default directory

(2) file `PS_LOCALINIT.COM` in the current login directory (as defined by logical name `SYS$LOGIN`)

(3) file `PS_EXE:LOCAL.COM`

The first file to be found, if any, is the only one to be run.

Thus, by placing `PS_LOCALINIT.COM` files in different locations, different sets of logical names may be used for different purposes.

If the user does not supply a `PS_LOCALINIT.COM` file, and file `PS_EXE:LOCAL.COM` exists, this file will be run. This file can be used to supply local initialization options for the Powder Suite.

A "news" file, `PS_EXE:PSNEWS.INIT`, is displayed each time the package is initialized, if this file exists. This file is intended to alert users to updates or other changes in the programs.

5.1 Local command file

The person installing Powder Suite may create a command file, PS_EXE:LOCAL.COM, to set the logical names used by the Powder Suite programs. If this file exists, and there is are no PS_LOCALINIT.COM files in a user's default or login directory, this file may be used to establish a menu of options for defining these logical names. A typical application for use of this file would be to offer the user a choice of hard-copy graphics devices.

An example local command file is shown below. In this case the user is able to choose between a PostScript laser printer (on a remote computer) and a pen plotter attached to the local system. Additional examples may be found in the PS_EXE: directory.

```
$   if F$TRNLNM("ps_hdev") .nes. "" then deass ps_hdev
$   if F$TRNLNM("ps_hfile") .nes. "" then deass ps_hfile
$   if F$TRNLNM("ps_hcom") .nes. "" then deass ps_hcom
$   if F$TRNLNM("PGPLOT_HPGL_SPEED") .nes. "" then deass PGPLOT_HPGL_SPEED
$   inquire ans "Use LASER plotter for graphics? (Y/[N])"
$   if .not. ans then goto HP
$   define ps_hfile plot.ps
$   define ps_hdev ps
$   define ps_hcom "@sys_com:lasersub ps_hf_last"
$   exit
$ HP:
$   WRITE SYS$OUTPUT "Using HP plotter for graphics"
$   define ps_hdev hpgl
$   define ps_hfile hp_plotter:
$   inquire ans "Use 11x17 inch paper (Y/[N])"
$   DEFINE/NOLOG PGPLOT_HPGL_PAGE B
$   if .not. ans then DEFINE/NOLOG PGPLOT_HPGL_PAGE A
$   inquire ans "Enter pen speed in cm/sec (1-38) [default=max]"
$   if ans .nes. "" then DEFINE/NOLOG PGPLOT_HPGL_SPEED 'ans'
```

5.2 Local help file

Entries with help information for local users can be included in the Powder Suite help library by creating file LOCAL.HELP in the [.PS] directory. If this file is found when the HELP.COM procedure is run, these help entries will be included in the help library. The LOCAL.HELP file should have standard VMS format: use a number in the first column followed by the help entry name; use 1 for a main entry, 2 for a sublevel entry and so on...

```
1 WHERE_IS_IT
  Powder Suite is installed in DISK11:[PS]
1 Problems
  In case of problems read the manual, get a copy from...
2 Serious_problems
  Contact ...
```

After modifying or creating the LOCAL.HELP file, run @HELP to create a new copy of the help libraries accessed by the programs.

5.3 Interactive/Hardcopy devices

The Powder Suite package can access up to four different I/O devices, none of which are required for operation.

(1) The interactive terminal is used for input of commands and output of responses by the package. This will not exist for batch mode operation of the program.

(2) The interactive graphics display device will usually be the same as the interactive terminal. It is possible (and perhaps optimum) that a separate device be used for graphics, but allocating two terminals, one for graphics and one for text, to the same login session requires system-level intervention and is rarely done; it will not be discussed here.

(3) The hardcopy graphics output device, may be a laser printer, plotter or any other supported graphics device. Output is typically written to a file and a DCL command or command procedure is used to spool the file to the actual device. Output can be sent directly to a device, if desired.

(4) The printer is used for hardcopy of text output from the programs. Any 132 column printer may be used. Output is again typically written to a file and then spooled.

It is likely that different users will choose to use different terminals, printers and plotters. If so, users will desire to customize the setup of the program for their preferences. This is done by creating a `PS_LOCALINIT.COM` file in either their default or login directory.

5.4 Logical names

The following logical assignments must be defined to use Powder Suite:

`PS_EXE` is the location of the `.EXE`, the `.HLB` files, and the `.COM` files for the package. This will be determined by where the package has been installed. (File `PS.COM` can be located anywhere convenient, but be sure the definition of `PS_EXE` in the `PS.COM` file is correct.) Include a disk assignment in the definition of PS_EXE, even if your system only has one disk.

`PS_JCPDS` and `PS_BITMAP` are the locations of the PDF-1 JCPDS-ICDD database files.

`PS_PDF2_CDROM` or `PS_PDF2_DISK` and `PS_PDF2_INDEX` are the locations of PDF-2 JCPDS-ICDD database files. The actual devices will be determined by where the package is installed.

`PS_TMP` is a device/directory for scratch files. Use the system scratch disk if one exists and it is regularly cleaned up. Otherwise define `PS_TMP` as `SYS$LOGIN` or `SYS$SCRATCH`.

`PS_CRT` contains an integer value which defines the terminal type and its graphics capability. The menu of choices is displayed when the package is initialized, unless a definition is supplied within a `PS_LOCALINIT.COM` or a `PS_EXE:LOCAL.COM` file.

`PGPLOT_FONT` and possibly `GRPCKG` are needed for the PGPLOT graphics package. `PGPLOT_FONT` must be defined as the location of the PGPLOT font file, `GRFONT.DAT`. If the PGPLOT shareable library has been used to link the programs, `GRPCKG` must point to file `GRPSHR.EXE`.

The following definitions are not required, but their use is recommended:

`PS_HDEV`, `PS_HFILE` and `PS_HCOM` determine the where hardcopy graphics should be directed. `PS_HDEV` defines the type of graphics device, (as defined in PGPLOT); `PS_HFILE` defines the default plot file name and `PS_HCOM` defines a command that can be used to process or queue the file (see the following examples). Note that each time a graphics file is created, logical name `PS_HF_LAST` is defined by the package as the full name of the graphics file that was actually written.

`PS_PFILE` and `PS_PCOM` define a file to be used for a hard copy printer and an optional command to process/queue the print file after it has been written. They are used the same manner as `PS_HFILE` and `PS_HCOM` (see the following examples). The logical name `PS_PR_LAST` is defined by the package as the full name of the print file that is actually written.

The following definitions are not required, but can be used to tailor the package to an inividual user's preferences.

`PS_WAVELENGTH` defines the default mode used in the programs, for example, when displaying JCPDS-ICDD entries: d-space or 2θ and in the latter case defines the wavelength that for conversion. If this logical is not assigned, the default is d-space mode. To use a different default, this logical name may be defined in a `LOGIN.COM` file or a user's `PS_LOCALINIT.COM` file. Once the wavelength setting is changed within a program, the logical name will (re)assigned for the remainder of the login session.

`PS_DELETED` defines the default mode used in the programs for processing of deleted patterns. Use command

```
$ DEFINE PS_DELETED TRUE
```

to cause "deleted" patterns to be used by default.

5.5 Examples

Some typical examples for logical name definitions are given below, along with explainations.

5.5.1 Terminal Type Definition

If a user will only access one type of terminal, it may be desireable to define the terminal type in the user's `PS_LOCALINIT.COM` file. Use command:

```
$ DEFINE PS_CRT "1"
```

to define `PS_CRT`. Note that the number should be defined between quotation marks with no extra spaces following the last digit.

5.5.2 Graphics Device Type Definition

Commonly users will wish to override the default graphics device settings. For a list of the currently defined devices, see file `CURRENT.DRIVERS` in the PGPLOT directory. Note that the "/" preceding the device name is omitted: `PS` for `/PS`. Some sample definitions are given below:

(1) This example uses PostScript output and a locally defined command procedure to process the file after creation.

```
$ DEFINE  PS_HDEV   PS
$ DEFINE  PS_HFILE   PLOT.PS
$ DEFINE  PS_HCOM   "@local_dir:postprocess PS_HF_LAST"
```

(2) This example uses QUIC output for a QMS or Talaris laser printer and then sends the output directly to the printer.

```
$ DEFINE  PS_HDEV   QMS
$ DEFINE  PS_HCOM   "PRINT/QUE=LASER/DELETE PS_HF_LAST"
```

(3) This example sends HPGL code to an Hewlett Packard plotter. The output is sent to the plotter as it is created.

```
$ DEFINE  PS_HDEV   HPGL
$ DEFINE  PS_HFILE   sys$plotter:
```

5.5.3 Printer Device Definition

(1) This example uses the default file name, and prints it on the system printer. This example is typical for most users who may wish to change the `/FORM=` or add `/QUE=` or other similar qualifiers.

```
$ DEFINE  PS_PCOM   "PRINT/FORM=132COL/DELETE PS_PR_LAST"
```

(2) In this example print files will be named `PS.PRINT` and will be printed by command procedure `LOCAL_DIR:POSTPRINT.COM`.

```
$ DEFINE  PS_PFILE   PS.PRINT
$ DEFINE  PS_PCOM   "@local_dir:postprint PS_PR_LAST"
```

5.5.4 D-Space/2θ Mode Definition

(1) set mode to 2θ angles with Cu Kα_1 radiation as the default

```
$ DEFINE  PS_WAVELENGTH  CU1
```

(2) set mode to 2θ angles with wavelength = 1.23456Å

```
$ DEFINE  PS_WAVELENGTH  1.23456
```

(3) set mode to d-space

```
$ DEFINE  PS_WAVELENGTH  0.0
```

5.5.5 "Deleted" Pattern Mode Definition

(1) set mode as using "deleted" patterns as the default mode on startup

```
$ DEFINE  PS_DELETED  TRUE
```

(2) set mode as not using "deleted" patterns as the default mode on startup

```
$ DEFINE  PS_DELETED  FALSE
```

Chapter 6: Installation Instructions

This chapter gives instructions for loading the Powder Suite package onto a VAX/VMS system. The programs have been tested on systems running VMS version 4.7 through 5.4; the package will likely run under all 4.x versions but probably will not run on VMS version 3.x or earlier. It is recommended that the programs be relinked on your local system during installation and after each operating system upgrade.

If bugs are found in these programs please document them as best possible and notify Brian Toby. If you want a rapid solution to the bug, you may be best off trying to fix it yourself. Bugs, particularly with fixes, will be greatly welcomed by the authors. Suggestions for additional features will not be quite so well received.

DCL procedures have been written to simplify installation. Most users will be able to load, install and rebuild the programs by following the few steps in the following section and answering the few questions asked during the installation procedure.

6.1 Summary of Installation Instructions

(0) Before starting to install the software, decide the following items:

- (A) Where will the software be placed: which device and which directory? Replace `dev:[dir...]` in the following steps with this information. For example: `USER:[XRD...]` to put the files in the XRD "account" or `DUA0:[000000...]` to create root-level directory `DUA0:[PS...]`.
- (B) Which version of the PDF-2 (full) JCPDS-ICDD database will be used? Your choices are on disk, on CD-ROM or none. Where will this file be placed?
- (C) What graphics devices are available on your system? What printers are available? Which printer and plotter should be the default device for users to send their output? What DCL commands will be needed to process or queue the files?

(1) Load the PS software/PDF-1 database/graphics library from tape

```
$ BACKUP  mua0:/SAV/REW dev:[dir...]/NEW_VERSION
```

(2) Install the PDF-2 (optional – see below)

(3) Use the installation procedure to link the code and create the appropriate `.COM` files.

```
$ SET DEF dev:[dir.PS]
$ @INSTALL
```

(4) Test the package.

```
$ SET DEF dev:[dir.PS]
```

`$ @PS` – (try out HELP, LOGIC and SEARCH, test out as many options as possible)

6.2 Required Directories and Files

The package is distributed as two savesets on a single tape. The first saveset contains the Powder Suite software, including all source files and object files. Also included in the first saveset is a partial distribution of the graphics package used in the programs (PGPLOT) and the PDF-1 JCPDS-ICDD database files.

The second saveset contains source code and documentation for the graphics package. This saveset need not be loaded, but may be of use to more advanced users. If the PDF-2 files will also be used with these programs, a CD-ROM or a set of tapes with the PDF-2 database must also be obtained from the JCPDS-ICDD.

The tape obtained from the JCPDS-ICDD may not be distributed to anyone other than the intended receipient, since duplication and distribution of this tape would violate your copyright agreement with the JCPDS-ICDD. The Powder Suite software, without the database, may be distributed subject to the restrictions given at the copyright notice, above.

To run this package, you will need the files described in the following sections of this documentation. They consist of:

(1) The Powder Suite Files

The only Powder Suite program files that are required to be kept on-line are the `.HLB`, `.EXE` and `.COM` files found in the `[PS.EXE]` directory plus file `PS.COM` in the `[PS]` directory. The logical name `PS_EXE` will be needed to define the location of executable files. Other files that are needed to run the programs are: the PGPLOT Graphics library, usually located in the `[PS.PGPLOT]` directory; the PDF-1 files, usually located in directory `[PS.PDF1]`; if the PDF-2 database is used, the three files in directory `[PS.PDF2]`.

(2) The Graphics Package

At a minimum, you will need to have the font table, file `GRFONT.DAT` on-line. Logical name `PGPLOT_FONT` will define the location of this file. To relink the programs you will also need the non-shareable object library, `GRPCKG.OLB` or the shareable image files, `GRPSHR.EXE` and `GRPSHR.OLB`. If you use the shareable image version (recommended), you will use logical name `GRPSHR` to define the location of the `GRPSHR.EXE` file.

These files may be located on any on-line disk in any directory where users of the programs will have read access. As distributed, a subset of the PGPLOT files are located in directory `[PS.PGPLOT]`.

(3) The JCPDS-ICDD Database

PDF-1:

A copy of the JCPDS-ICDD PDF-1 database is required to run LOGIC and SEARCH. The PDF-1 files must be in the Harlow/Toby modification of the format developed by Goehner and Garbauskas. These PDF-1 files optionally may be used in CMPR and MANIP. This database is copyright by the International Centre for Diffraction Data and may be only used with a license.

The PDF-1 files can be located in any directory on any on-line disk where users of the programs will have read access. Two logical names `PS_JCPDS` and `PS_BITMAP` are used to define the location of these files. As distributed, both sets of files are located in directory `[PS.PDF1]`.

The PDF-1 files are build using the ENCODE programs from the PDF-2 database. The ENCODE programs may also be used to include locally defined entries in the database.

PDF-2:

Program LOGIC can access the PDF-2 database from CD-ROM or from a disk file, but the PDF-2 file is not required for program LOGIC. Program SEARCH does not access the PDF-2 database.

6.3 Loading The Source Code

For the command procedures for compiling/linking and installation to work properly and for convenience, it is strongly suggested that you retain the directory structure used in the backup saveset.

To restore the PS saveset, use the command:

```
$ BACKUP  mua0:/SAV/REW dev:[dir...]/NEW_VERSION
```

where `dev:[dir]` is the directory where the package is to be placed. This creates subdirectory `dev:[dir.PS]` and a number of "sub-subdirectories", for example `dev:[dir.PS.EXE]`. Use of this command will retain the original directory structure. If it is desired to move all the files or use a name other than `[dir.PS...]`, the file `dev:[dir]PS.DIR` can be renamed. To create PS as a root directory, use `dev:[000000...]`.

Note that the name `mua0:` will need to be replaced with the appropriate device name for your system, such as `MSA0:`, `MKA500:`, or `$TAPE1:`

Likely, it will be most convenient to keep the source and object files on-line, since they require only around 5,000 blocks. However, you can delete either the source files or the object code (or both) after installation. The only files that must be retained are described in the previous section. Note that command files `DELOBJECT.COM` and `DELSOURCE.COM` are provided for deleting the source and object code, respectively.

6.4 Plotting Package

After loading the PS files, the full PGPLOT/GRPCKG graphics library can optionally be loaded. This is not required, but is recommended for users who wish to "get their hands dirty" and optimize the installation for their own site, or modify the code, or write a graphics driver for an unsupported device (often not very difficult!). The package is quite easy to use and may be valuable to users on your system for their own programming.

For best performance and the smallest `.EXE` files you should use the shareable image version. (See Appendix C in the PGPLOT documentation files for more info.) No system privileges are needed to install the package as a shareable image. Note that if the shareable image will be used, an extra file (`GRPSHR.EXE`) must remain on-line and an extra logical name (`GRPSHR`) will be used. If the shareable image is used, then support for additional graphics devices can be added without recompiling the Powder Suite programs. The main disadvantage is that the shareable library should be relinked on each system (or cluster) where it will be used and should probably be relinked after each operating system upgrade.

A subset of the full PGPLOT distribution is contained in subdirectory `[.PS.PGPLOT...]`. If the full package will be loaded, for simplicity it is recommended that the files are placed in a subdirectory `[.PS.PGPLOT...]`, using restore command

```
$ BACKUP  mua0:/SAV/NOREW dev:[dir.PS...]/NEW_VERSION
```

There are many command files in the `[.PGPLOT]` directory for partial or complete rebuilds of the package. The most simple to use is procedure `PGINSTALL.COM` in the `[PS]` directory, which selects supported graphics devices, recompiles and relinks all code. That procedure calls routines `CHOOSE.COM`, `COMPILE.COM`, `BUILD.COM` and `LIST_DRIVERS.COM`. Note that if drivers are added to the PGPLOT library, the Powder Suite programs need to be recompiled, unless the shareable image version of PGPLOT has been used.

This package is copyright and is distributed with permission of the author, Tim Pearson of the Caltech Astronomy Department, on the provision that any software based on his package be distributed without a fee.

If the shareable image is used, the following logical definitions will be needed:

to run:

```
$ PGPLOT   := $disk1:[public.pgplot] ! system dependent
$ DEFINE PGPLOT_FONT     'PGPLOT'GRFONT.DAT
$ DEFINE GRPSHR          'PGPLOT'GRPSHR.EXE
```

to link:

```
$ DEFINE LNK$LIBRARY     'PGPLOT'GRPSHR.OLB
```

As distributed, the `.EXE` files are linked without using the shareable image version of the library, since this is more portable. The logical assignments are then:

to run:

```
$ PGPLOT   := $disk1:[public.pgplot] ! system dependent
$ DEFINE PGPLOT_FONT     'PGPLOT'GRFONT.DAT
```

to link:

```
$ DEFINE LNK$LIBRARY     'PGPLOT'GRPCKG.OLB
```

These definitions can be put in the system startup files, login startup files. The are usually located in the `PS_LOCALINIT.COM` file of the PS package (described later).

6.5 JCPDS-ICDD Files

The JCPDS-ICDD database consists of the following group of files:

```
CHEM.BITMAP;1          1300
DI.LIBRARY;1          15093
DSP00.BITMAP;1         3273
DSP30.BITMAP;1         3273
DSP3S.BITMAP;1         3273
DSP70.BITMAP;1         3273
ELMCOUNT.BITMAP;1       100
JCPDS.INDEX;1          1599
MISC.BITMAP;1           100
NAME.DIRECT;1          7675
```

Note that the actual sizes of these files varies with the version of the database, the use of deleted patterns and the number of local patterns which are added to the database.

A license from the JCPDS-International Centre for Diffraction Data is required for use of these files. Logical names PS_JCPDS and PS_BITMAP must be defined with the location of these files. Logical name PS_BITMAP points to the location of the .BITMAP files, while logical name PS_JCPDS points to the remaining files.

If Powder Suite will run on more than one computer (or cluster), the PS_JCPDS files may be accessed across a DECNET link and thus stored on a single VAX, however this will slow database access and is not recommended. The programs have never been successfully run where the PS_BITMAP files are accessed via DECNET.

If the PDF-2 database will be accessed by program LOGIC, either on disk or on CD-ROM the following files are also be required:

```
CODENS40.DAT;1        266
DISP.INIT;1             1
MINERAL40.DAT;1        24
VAXPDF40.BIN;1          7
```

Note that in later releases the set number (40) may increase and the file sizes may also change. These files are provided by the JCPDS-ICDD for use with the PDF-2 database.

Logical name PS_PDF2_INDEX must be defined with the location of these files. While it is possible to access the files across DECNET, again this is not recommended.

If the PDF-2 file will be accessed by LOGIC on disk, logical name PS_PDF2_DISK should be defined to point to the directory containing the file:

```
JCPDS.DIRECT;1       255613
```

Access of this file over DECNET has been tested and while it does result in somewhat slower access, it is often faster than CD-ROM access and may well be worth the savings in disk space.

If the PDF-2 file will be accessed by LOGIC on CD-ROM, the disk should be mounted from a system-level account using the following command.

```
$ mount/for/sys/prot=(s:REWD,o:REWD,w:REWD,g:REWD) DUB0
```

If the CD-ROM will be mounted on a device other than DUB0:, logical name PS_PDF2_CDROM should be defined to point to this device. The CD-ROM version of the PDF-2 may be shared on a cluster, provided that the drive appears to be local to each system on the cluster, but the CD-ROM drive cannot be shared via DECNET.

Program LOGIC can be used with either version of the PDF-2, or without the PDF-2 database. The program checks for definition of logical names `PS_PDF2_DISK` and `PS_PDF2_CDROM` to see if a PDF-2 file is available.

6.6 Compiling and Linking the Powder Suite

The executable files on the distribution saveset may not run properly on your system if you have an earlier version of VMS than the one used for the distribution copy of the programs, so it is recommended to relink during installation. This will be done by the `INSTALL.COM` command procedure as a default option. Other routines will be useful to people wishing customize or expand the programs or documentation.

Supplied command files in directory `[.PS]`:

`INSTALL.COM`

A fairly user-friendly routine for installing and linking the PS package. Checks for required files and relinks. Calls `SELPDF2.COM`, `WRINIT.COM`, `PGINSTALL.COM` and `CLEANUP.COM` and other files.

`HELP.COM`

Creates the main help files (`PS.HLB`) from the `.TEX` documentation files. If file `LOCAL.HELP` is found in the current directory this file is included in the help library. Also creates ASCII (`.DOC`) versions of the TEX documentation.

`CLEANUP.COM`

Deletes unneeded files.

`SELPDF2.COM`

Selects the version of the PDF-2 database to be used.

`WRINIT.COM`

Writes the `PS_INIT.COM` file with logical definitions used to initialize the package.

`WRLINIT.COM`

Can be used to write a `PS_LOCALINIT.COM` file with logical definitions to initialize the package.

`DELOBJECT.COM`

Deletes all object code files (`.OBJ`) and object code libraries (`.OLB`). This will save around 2,000 blocks at the expense of some computer time, if it is ever necessary to relink the package. Note that it will not be possible to rebuild these files if your system does not have a FORTRAN compiler.

`DELSOURCE.COM`

Deletes all FORTRAN and TEX source and object code, and most command files. This will save around 4,000 blocks. However, it is not recommended to perform this action unless disk space is very tight as you may wish to rebuild some of the code at some future time.

MASTER.COM

Used to recompile and link all programs and rebuild their help files. Calls HELP.COM.

RELINK.COM

Used to relink all programs using the existing object libraries.

PGINSTALL.COM

Facilitates the configuration, compiling and build libraries for PGPLOT.

PGLNKLIB.COM

Specifies the location of the PGPLOT graphics library. Created by PGINSTALL.COM; called as needed by the Link command files. Should never need to be called directly or edited.

GSASLNKLIB.COM

Specifies the location of the GSAS object library. If GSAS is actively used and upgraded, it is best to modify this file to reference the file GSASLIB.OLB supplied by Los Alamos on their distribution tape.

MAKEGSASLIB.COM

Used to update the subset of the GSAS object library used by PS. Before using the file, it must first be edited to specifies the location of the GSAS object library. This need only be used when GSAS is upgraded. It is better to modify GSASLNKLIB.COM so that the the file GSASLIB.OLB supplied by Los Alamos is used for linking.

6.7 Installation of Command Procedures

Two DCL command procedures are used to run the package:

XRD:[PS.EXE]PS_INIT.COM and XRD:[PS]PS.COM.

The first time the PS command procedure (PS.COM) is used, and any time the command procedure is used with the INIT option, the DCL procedure executes the system-wide definitions found in the [PS.EXE]PS_INIT.COM file. In addition, users may supply override these definitions with their own PS_LOCALINIT.COM file. The PS command procedure looks for a file named PS_LOCALINIT.COM in:

(1) the current default directory

(2) the current login directory (as defined by SYS$LOGIN)

If neither of these files are found, and a PS_EXE:LOCAL.COM file is found, this file is executed. This file may be used to provide a menu of setup options. See the Customization chapter for more information.

When INSTALL.COM is used, it creates the PS_INIT.COM file and updates the definition of logical name PS_EXE in file PS.COM. If for some reason INSTALL.COM is not used, this definition must be updated. In addition the definitions of the following logical names must be properly defined in file PS_INIT.COM.

PS_EXE is the location of the .EXE, the .HLB files, and the .COM files (file PS.COM can be located anywhere convenient).

PS_JCPDS and PS_BITMAP are the locations of the PDF-1 JCPDS-ICDD database files. PS_PDF2_CDROM or PS_PDF2_DISK and PS_PDF2_INDEX are the locations of PDF-2 JCPDS-ICDD database files.

PGPLOT_FONT and possibly GRPCKG are needed for the PGPLOT graphics package.

PS_TMP is a device/directory for scratch files.

PS_HDEV and PS_HFILE determine the default graphics hardcopy device type (as defined in PGPLOT) and the default plot file name. A command to process the file can also be defined as PS_HCOM

PS_PFILE and PS_PCOM define a file to be used for a hard copy printer and an optional command to process/queue the print file after it has been written. The are used the same manner as PS_HFILE and PS_HCOM

6.8 Upgrading the Database

A new release of the database is generated each year by the ICDD. To replace the old version of the database with the new version requires replacing The PDF-2 database with the newer release and loading or rebuilding the PDF-1 files from the new PDF-2 files.

If the PDF-2 is obtained from the ICDD on CD-ROM, loading the PDF-2 database simply means placing the new CD-ROM into the CD drive. Loading the PDF-2 database to disk is a more difficult task, requiring that the file be copied from tape or CD-ROM to disk. Program COPYCD in the [.ENCODE] is provided to copy the PDF-2 database from CD-ROM to disk, optionally removing deleted patterns. Program CDCOPY may be used to copy any file from the CD-ROM and program CDDIR is used to list the contents of the database. To load the files from magnetic tape, the BACKUP command is normally used. Instructions are usually supplied with the tape.

The four files in directory [.PS.PDF2]: DISP.INIT, CODENSxx.DAT, MINERALxx.DAT and VAXPDFxx.BIN are created by the ICDD with each release of the database, where xx is the most recent set number in the release. It is suggested that you update these files with upgrade of the database, but this is not required. Note: all four files must be replaced at the same time.

Future releases of the PDF-2 on CDROM may possibly include the Powder Suite PDF-1 files. If so, instructions will be distributed with the CD-ROM on how to copy these files from the disk.

The PDF-1 files may be built from the PDF-2 database using the ENCODE programs or may be obtained from the ICDD. If the PDF-2 database will not be used, the database must be obtained in PDF-1 format rather than PDF-2 format.

6.9 Upgrading the Software

To upgrade the software from previous versions of Powder Suite, you may load the new files into the same directories as the same previous version. If so, be sure to use the /NEW_VERSION option for the BACKUP command. If the same directories are used, the old version of the program may not be accessed once the upgrade is started.

If space allows, it is also possible to load the Powder Suite files in a second location, build the programs (and possibly the PDF-1 database), test the new package and then delete the old version. If the package will be moved (most easily by renaming the PS.DIR file), it will be necessary to rerun the INSTALL.COM procedure after moving the files, but to save time, do not recompile or relink the programs.

The version of Powder Suite released with Set 41 of the database will not function with older versions of the PDF-1 files. If this version of the software will be used with a previous version of the database, it is necessary to rebuild the PDF-1 database files from the PDF-2 database using the ENCODE programs.

Chapter 7: Programmer's Information

7.1 Source Code

The LOGIC, SEARCH and ENCODE programs consist of a large number of subroutines which are found in the appropriate directories. The subroutines in the `[.RET3]` routines are also used in LOGIC and ENCODE for access to PDF-2 database. All programs use other subroutines found in the `[.SHARED]` directory.

Routine `BUILD.COM` in each directory is used to compile and link the programs. This file in turn calls other files used to build and interprete the command definition language (`.CLD`) file, compile the program(s), build an object file library and finally link the program(s).

7.2 Documentation/Help File Format

There are five on-line help libraries, `PS.HLB`, `LOGIC.HLB`, `SEARCH.HLB`, `CMPR.HLB`, and `MANIP.HLB`. These files may be accessed with the command:

`HELP/LIBR=PS_EXE:PS` (etc.)

or by typing `@PS HELP` (or `PS HELP`). Help is also available from inside the CMPR, LOGIC, SEARCH and MANIP programs by typing HELP, optionally followed by a command name.

The online help files (`.HLP`) are encoded, along with the command definition language (`.CLD`) files into TeX documentation files (`.TEX`). These files have a simple, fixed format which allows a single file to be used for three different purposes. The `.TEX` files can be processed by the TeX typesetting language (see The TeXbook, D. Knuth, Addison Wesley) with no preprocessing. However, since two simple editing procedures are used to convert the files to `.CLD` and `.HLP` format, the number of TeX commands should be restricted to those listed in the following paragraphs.

Documentation format: (angle brackets, `<` and `>`, delimit items that must be specified.

```
%CLD%Module <program>_SUBCOMMANDS
%CLD%
\Program <program>
%HLP%1 HELP
%HLP%               Information on commands within <program>
  %CLD% <... definition of 1st command ...>
%CLD%
\Command <name of 1st command>\par
<... description of command goes here ...>
\Parameter
\parm
parameter <name>\par
<... a description of the parameter(s) goes here ...>
\Qualifiers
\qual
<qualifier number 1>\<
<qualifier number 2>\<
<last qualifier>\par
```

```
<... a description of the qualifier(s) goes here ...>
\Examples
\exam
<line with an example>\par
<... a description of the example goes here ...>
 .
 .
 .
```

Lines beginning with `%CLD%` will be copied to the `.CLD` file and the `%CLD%` prefix will be removed. This prefix should appear at the beginning of each line. (Lines with this prefix will be ignored by TeX).

The `.HLP` file is copy of the `.TEX` file except for the following changes: The `%HLP%` prefix will be removed from lines so that will be used in the `.HLP` file, but will be ignored by TeX. Lines beginning with `\!` will be used in the TeX file, but will be removed from the `.HLP` file.

The `\Qualifier`, `\Parameter`, `\Example` lines are translated to the appropriate headers for Help library format, but they must start in the first column. The `\Program` line is translated to a comment line.

Lines containing `\qual`, `\exam`, `\parm` and `%CLD%` are removed from the `.HLP` file.

The following TeX codes are translated: (` `` `) becomes (`"`); (`''`) becomes (`"`) and (`\#`) becomes (`#`). The following codes are removed: `\<`, `\par`, `{`, and `}`

The following definitions are used for TeX special symbols and are translated to the string in parenthesis:

`\Kalpha1` (`K alpha 1`),

`\Kalpha2` (`K alpha 2`)

`\twotheta` (`two-theta`)

`\muVAX` (`microVAX-II`)

`\TAB` (two spaces)

Chapter 8: The ENCODE programs

8.1 Description of Programs

The ENCODE programs are a package of four programs which create the condensed (PDF-1) database files and index files needed by Powder Suite. The first program, PDF1, creates the PDF-1 data files from the full (PDF-2) JCPDS-ICDD database along with an index to the PDF-1 and PDF-2 database files. The second program, ADDPDF1, is used to add PDF-1 format entries to the PDF-1 files written by program PDF1. These entries are easier to prepare than PDF-2 entries. The third program, WRDI, is used to create the d-space index files which are used for rapid searching of the database by peak position and the fourth program, WRCHEM, is used to create the elemental composition index files which are used for rapid searching of the database by chemistry.

The programs must be run in sequence, but the second program, ADDPDF1, may be omitted unless it is desired to add additional PDF-1 entries into the local version of the JCPDS-ICDD database.

8.1.1 Program PDF1

The first program, PDF1, reads the PDF-2 database and creates a condensed subset of the original database called the PDF-1 database. The PDF-1 database consists of two files: NAME.DIRECT, which contains the chemical formula, chemical and mineral names; DI.LIBRARY, which contains the d-spaces (peak positions) and intensities for the peaks. Also written at this time is an index to the database, INDEX.DIRECT and an index to the various subfiles in the database, MISC.BITMAP.

Some users may wish to add their own entries to the database. If a file of AIDS*83 format entries (the format used in the PDF-2 database) is prepared, these entries may also be indexed by the PDF1 program and will be accessible by the Powder Suite programs identically with all other PDF-1 entries. Program LOGIC as both PDF-1 and PDF-2 entries. A copy of the PDF-2 database licensed by the ICDD is required to run this program.

8.1.2 Program ADDPDF1

The second program, ADDPDF1, is used to add PDF-1 format entries to the PDF-1 files written by program PDF1 (NAME.DIRECT, DI.LIBRARY, MISC.BITMAP and INDEX.DIRECT). These entries contain much less information than is required in a PDF-2 entry and are easier to prepare. This program does not require access to a PDF-2 database and thus may be used at locations where only the PDF-1 format database has been licensed.

Use of this program is optional and should be skipped if there are no PDF-1 entries to add. It is also possible to run ADDPDF1 more than once, adding additional entries with each subsequent run. Note that program PDF1 creates the PDF-1 database files from the PDF-2 database, while program ADDPDF1 adds new entries to the PDF-1 files. Thus, each time that program PDF1 is run, all PDF-1 entries must be added anew to the PDF-1 files using ADDPDF1.

8.1.3 Program WRDI

Program WRDI is used to create the d-space index files than are used for rapid searching of the database by peak position. These files consist of a single bit mapped to each database entry, the bit is set if the entry has a peak above the intensity threshold in the specified location. These files are also referred to as bitmap indices for this reason.

Two types of index files may be written by this program:

(1) a file that indexes the location of three strongest peaks in each entry, DSP3S.BITMAP

(2) a set of files that index the location of all peaks above an intensity threshold of `xx`%, DSP`xx`.BITMAP. The number of bitmap files that are created are at the descretion of the person who runs this program and the amount of available disk space. At a minimum files should be written with 0% and 70% thresholds. It is recommended that a 30% file be written, and that any other files be written at increments of 10%.

This program must be run after ADDPDF1 or PDF1 to update the index files.

8.1.4 Program WRCHEM

Program WRCHEM is used to create the elemental composition index file, file CHEM.BITMAP, that is used for rapid searching of the database by chemistry. This file consists of a single bit mapped to each database entry, the bit is set if the entry contains the specified element. This file is sometimes referred to as the chemistry bitmap index for this reason.

This program must be run after ADDPDF1 or PDF1 to update the index files.

8.2 Running the Programs

While the programs may be run interactively, they are fairly slow and cumbersome and will be most convenient to run as batch jobs. The following sections discuss the DCL logical names needed by each program and the input needed. Following the discussion, an example batch input file is shown.

8.2.1 Program PDF1

Program PDF1 requires the definition of several logical names for input and output:

`PS_PDF2_DISK`	The location of the PDF-2 disk file
`PS_PDF2_CDROM`	The location of the PDF-2 CDROM
`PS_PDF2_LOCAL`	The file with local PDF-2 additions to the database
`PS_PDF2_INDEX`	The location of the PDF-2 support files
`PS_JCPDS`	The directory where the PDF-1 files will be written
`PS_BITMAP`	The directory where MISC.BITMAP will be written

To run the program, one must define where the PDF-2 files will be located by either defining `PS_PDF2_DISK` or `PS_PDF2_CDROM` (not both). The default name for the PDF-2 file if on disk is JCPDS.DIRECT, if the file has some other name, the full file name should be specified, otherwise only the device and directory need be used. The file must be a 80-byte fixed record length file. Note that the disk file can be read via DECNET from another node. The default name for the CDROM is file name PDF2.DAT on device DUB0:; if both are true, then `PS_PDF2_DISK` does not need to be defined.

If the file is on another device, that device must be specified. Note that DECNET access to the PDF2 is not allowed, however sharing of the CDROM in a cluster may be possible.

Input is required to decide how to process "deleted" patterns in the PDF-2 database. While some patterns in the JCPDS-ICDD database are removed by the editors completely, some are flagged as "deleted" and a reference is given to the entries which specify the later entries which superceed these "deleted" patterns. Three options are available for processing of these "deleted" patterns.

(1) The patterns may be omitted completely from the PDF-1 database. If this is done, it is not possible to ever see the PDF-2 entries in program LOGIC. To do this enter a "N" on the first line of input.

(2) The patterns may have their chemical formula listed in the PDF-1 database but not their peak positions (d-spaces and intensities). If this is done it is possible to locate "deleted" entries based on chemical searches, but not on peak position searches and the PDF-2 entries may be displayed in program LOGIC. To do this enter a "Y" on the first line of input and a "N" on the second.

(3) The patterns may have both their chemical formula and peak positions listed in the PDF-1 database. If this is done, "deleted" patterns are processed largely the same as the other patterns. To do this enter a "Y" on the first line of input and a "Y" on the second.

The program also requires as input the expected sizes of the output NAMES.DIRECT and DI.LIBRARY files, in blocks. These numbers are used to reserve a block of space for each file. Note that there must be sufficient space on the disk to allocate files of this size, or the program will not run. All unused space will be released when the program ends. So, it is better to overestimate the space requirements, than underestimate them.

The three PDF-2 support files needed by PDF1 are `DISP.INIT`, `CODENSxx.DAT`, and `VAXPDFxx.BIN`, where xx is a set number (`40`, `41`, ...). The location of these files is defined using logical name `PS_PDF2_INDEX`. These files are produced by the JCPDS-ICDD for use with the PDF-2 database and are updated with each release of the database. If the files are updated, all three files should be updated together.

If local additions are to be supplied to the program, an 80-byte fixed record length file must be created with AIDS*83 format entries (see below). The entries must have card numbers above 99 and must have a set number of zero. Thus the entries must have be given numbers between 101 (0,0101) and 9999 (0,9999). The entries must be placed in the file sorted by order of increasing card number.

Sample batch input for program PDF1:

```
$ SET VER
$!  DCL procedure to create the PDF-1 files from the PDF_2 file
$ define PS_pdf2_index adisk:[toby.ps.pdf2]
$ define PS_pdf2_disk ESVAX::PUBLIC:[TOBY.SET39]
$ define PS_pdf2_local local.pdf2
$ define PS_JCPDS adisk:[toby.ps.pdf1]
$ define PS_bitmap adisk:[toby.ps.pdf1]
$ run adisk:[toby.ps.encode]pdf1
Y
N
10000
20000
$ EXIT
```

The following procedure is an example of a method which may be used to create a fixed length record file when creating the Local PDF-2 database.

```
$ SET VER
$!  DCL procedure to create a local PDF-2 file
$ create fixrec.fdl
FILE
ALLOCATION 0
BEST_TRY_CONTIGUOUS yes
EXTENSION 0
ORGANIZATION sequential
RECORD
BLOCK_SPAN yes
CARRIAGE_CONTROL none
FORMAT fixed
SIZE 80
$ convert/fdl=fixrec/pad   sys$input  adisk:[toby.ps.pdf2]local.jcpds
                                                       M          P   P000101X1
                                                    368.14      0.00  P000101X4
 0                                                                    P000101X5
Naphthylbismuth Dioxide (BHT)                                       P P000101X6
C10 H7 Bi O2                                                          P000101X7
C10 H7 Bi O2                                                          P000101X8
ANCHAM  10  475 1938 Foo, Bar et al.                                  P000101X9
MoKa1 0.709        F        DD        X 16.0                          P000101XF
X                     BB                                              P000101XG
20.0000000            9.90000 18            3.40000  5               1P000101XI
3.22000  3            3.15000  3            2.98000  3               2P000101XI
2.67000 10            2.06000  3            1.93000  5               3P000101XI
1.88000 10            1.61000  5            1.57000  3               4P000101XI
1.52000  3            1.33000  3            1.24000  3               5P000101XI
1.19000  5                                                           6P000101XI
                  EGS 85/ 1/13  0  0 08 84/12/13                      P000101XK
$ del fixrec.fdl;
$ exit
```

8.2.2 Program ADDPDF1

Program ADDPDF1 requires the definition of two logical names for input and output:

- `PS_JCPDS` The directory where the PDF-1 files will be read and written
- `PS_BITMAP` The directory where MISC.BITMAP will be read and written

The program reads files NAMES.DIRECT, DI.LIBRARY, JCPDS.INDEX and MISC.INDEX and writes new files in the same directories.

The program requires as input the expected sizes of the output NAMES.DIRECT and DI.LIBRARY files, in blocks. These numbers are used to reserve a block of space for each file. Note that there must be sufficient space on the disk to allocate files of this size, or the program will not run. All unused space will be released when the program ends. So, it is better to overestimate the space requirements, than underestimate them.

The PDF-1 additions must also be supplied to the program as a set of lines for each entry. Card numbers must be above 99, as before, but there is no upper limit for the entry numbers. It is recommended, however, that numbers not exceed 9999, so that local entries do not replace entries in the database. The entries must be input sorted in order of increasing card number. If desired, this program may be used to enter new PDF-1 entries for existing PDF-2 entries, thus overriding the entries in the ICDD-JCPDS database.

A PDF-1 entry consists of the following free-format lines of input.

A) card number
B) chemical formula
C) chemical name
D) number of peaks, reference intensity (I/Ic)
E) pairs of d-spaces and intensities (one or more pairs per line)
F) subfile flags

The chemical formula should consist of element symbols followed by an element count. If a mineral name is to be specified, it should follow the chemical name, separated by a slash. Up to 200 peaks may be specified for an entry. Peak positions should be given as d-spaces (in Å) and peak intensities are relative and will be scaled by the program so that the strongest peak is 100%. The subfile flags may be one or more of the following numbers:

1 Inorganic
2 Organic
3 Common Phases
4 Minerals
5 Alloy/Metal/Intermetallic
6 NIST (NBS)
7 Forensics
8 Zeolites
9 Deleted patterns
10 Local patterns (always set)

All subfile flag values must be on one line, separated by commas.

Sample batch input for program ADDPDF1:

```
$ SET VER
$ set def adisk:[toby.ps.PDF1]
$!  DCL procedure to add PDF-1 entries to the main PDF-1 files
$ define PS_JCPDS adisk:[toby.ps.pdf1]
$ define PS_bitmap adisk:[toby.ps.pdf1]
$ run adisk:[toby.ps.encode]addpdf1
15000
25000
201
Al2 O2
gamma-Alumina (Toby)
5
20.0, 10
10.0, 50
5.0, 100
4.0, 40,   3.0, 20
```

```
1,3,4
202
Al2 02
delta-Alumina (BHT)
2
20.0, 50
10.0, 50
1,3,4,9
-1
$ PURGE adisk:[toby.ps.pdf1]*.*
$ EXIT
```

8.2.3 Programs WRCHEM and WRDI

Programs and WRCHEM and WRDI require the definition of a logical name for input and a second one for output:

`PS_JCPDS` The directory where the PDF-1 files will be read
`PS_BITMAP` The directory where bitmap files will be written

Programs and WRCHEM and WRDI are most commonly run together in a single batch run. No input is required for WRCHEM. Program WRDI requires a set of input values that determines which bitmaps will be created by the programs. A value between 0 and 99 causes a index file to be created for all peaks with intensity greater than or equal to the specified value (where the strongest peak in the pattern is scaled to 100.) A value of -1 causes the program to write an index file to the "three strongest peaks."

Sample batch input for program WRDI and WRCHEM (in a single run):

```
$ SET VER
$! DCL procedure to create the JCPDS index files from the PDF-1
$ define PS_JCPDS adisk:[toby.ps.pdf1]
$ define PS_bitmap adisk:[toby.ps.pdf1]
$ run adisk:[toby.ps.encode]wrdi
-1
70
30
00
$ run adisk:[toby.ps.encode]wrchem
$ PURGE adisk:[toby.ps.pdf1]*.*
$ EXIT
```

Chapter 9: Summary of Command Formats

Program LOGIC

```
ADD (OR)
    /ELEMENTS=required_list
    /ELEMENTS
    /E_SPAN=req_range(s)
    /COUNT=elm_count
    /COUNT=(c_min,c_max)
    /COUNT
    /CARDS=card_list
    /CARDS
    /PEAKS=peak_list
    /PEAKS
    /ERROR=error_list
    /DSPACE
    /WAVELENGTH=wave_length
    /LEVEL=peak_level
    /EXACT
    /FAST
    /OR
    /AND
    /OPTIONAL=optional_list
    /O_SPAN=opt_range(s)

BROWSE

COMMENT  comment_line

CULL (NAND)
    /ELEMENTS=required_list
    /ELEMENTS
    /NOELEMENTS
    /E_SPAN=req_range(s)
    /COUNT=elm_count
    /COUNT=(c_min,c_max)
    /COUNT
    /CARDS=card_list
    /CARDS
    /NAME=compound_name
    /NAME=mineral_name
    /PEAKS=peak_list
    /PEAKS
    /ERROR=error_list
    /DSPACE
    /WAVELENGTH=wave_length
```

```
    /LEVEL=peak_level
    /EXACT
    /FAST
    /OR
    /AND
    /OPTIONAL=optional_list
    /O_SPAN=opt_range(s)

DCL

DELETED
    /INCLUDE
    /EXCLUDE

EXIT

FILE  file_name

HELP

INDEX
    /HANAWALT=sort_lines
    /HANAWALT
    /MAXD=sort_lines
    /MAXD
    /NAMES
    /PRINT

MATCH (AND)
    /ELEMENTS=required_list
    /ELEMENTS
    /NOELEMENTS
    /E_SPAN=req_range(s)
    /COUNT=elm_count
    /COUNT=(c_min,c_max)
    /COUNT
    /CARDS=card_list
    /CARDS
    /NAME=compound_name
    /NAME=mineral_name
    /PEAKS=peak_list
    /PEAKS
    /ERROR=error_list
    /DSPACE
    /WAVELENGTH=wave_length
    /LEVEL=peak_level
    /EXACT
    /FAST
    /OR
    /AND
    /OPTIONAL=optional_list
    /O_SPAN=opt_range(s)
```

```
READ  file_name
    /SUBPDF=sub_file
    /LIST=list_file
    /RANGE=(entry1,entry2)
    /OR
    /AND
    /NOT
    /REPLACE

TABLES
    /FULL

WAVELENGTH  wave_length
    /TARGET=target_type
    /TARGET
    /NOTARGET
    /WTYPE=wave_type

WRITE  file_name
```

Program SEARCH

```
DCL

DELETED
    /INCLUDE
    /EXCLUDE

EDIT

EXIT

FILE  file_name

HELP

IGNORE
    /DISPLAY
    /CARD=jcpds_card
    /CARD
    /IMIN=min_inten
    /INCLUDE
    /EXCLUDE
    /PEAK=position_list
    /PEAK
    /WIDTH=D_2THETA
    /RANGE=(min,max)
    /RANGE

LOAD  file_name

LOGIC

MATCH

QUIT

READ  file_name
    /FORMAT=fileform

REDUCE

REPORT
    /PRINT

SEARCH
    /BATCH
    /INTERACTIVE
    /PRINT

SET
    /Error=DEL_2THETA
    /R_INDEX=Req_Index
    /Rmin=R_Imin
    /F_INDEX=Forbid_Index
    /FWidth=FWHM
```

```
    /Fmin=F_Imin
    /MAXDBMISS=DB_max_miss
    /DB_IMIN=DB_min_int
    /MATCHOBS=OBS_min_lines
    /OBS_IMIN=OBS_min_int
    /MAXCARDS=MAX_hits
    /SORT=Num_Sort
    /SORT
    /NOSORT
    /FOM=Calc_type
    /NAME=search_name

SHOW

STARTFILE
    /LOGIC
    /USERPDF=file_name
    /SUBPDF=sub_file

TITLE

WAVELENGTH  wave_length
    /TARGET=target_type
    /TARGET
    /NOTARGET
    /WTYPE=wave_type
```

Program CMPR

```
ADD
    /TITLE="file_title"
    /SCALE=scale_factor
    /OFFSET=offset_val
    /MINIMUM

ATTRIBUTES
    /COLOR=color
    /WIDTH=width
    /LINE=line_type
    /PEAK=peak_type
    /OFFSET=off_value
    /MAGNIFICATION=mag_value
    /ALL

COMBINE  file_list

DCL

DEFAULT
    /AUTO
    /NOMANUAL
    /MANUAL
    /NOAUTO

DELETE  file_number
    /ALL

DGEN
    /A=a_length
    /B=b_length
    /C=c_length
    /ALPHA=bc_angle
    /BETA=ac_angle
    /GAMMA=ab_angle

EXIT

FILE  file_name

HKLPLOT
    /WIDTH=P_width
    /XLOW=low_limit
    /XHIGH=high_limit
    /DATASCALE=data_scale
    /PEAKSCALE=peak_scale

LOGIC

MANIP  file_number

PLOT  file_list
    /XLOW=low_limit
```

```
    /XHIGH=high_limit
    /Q
    /DSPACE
    /WAVELENGTH=wavel
    /STACK
    /NOSTACK
    /XSTACK=X_spacing
    /YSTACK=Y_spacing
    /RELATIVE
    /EXTREME
    /FIRST
    /YLOW=low_limit
    /YHIGH=high_limit
    /SIZE=(X_len,Y_len,X_mar,Y_mar)
    /SIZE=(X_len,Y_len)
    /SIZE
    /TITLE
    /NOTITLE
    /FILE
    /NOFILE
    /CLIP
    /LINEAR
    /LOG
    /SQRT
    /GRID
    /HARD

QUIT

READ  file_name

file_name_1, file_name_2,...  file_name_8
    /FORMAT=fileform
    /JCPDS=card_list
    /JCPDS

SCALE  file_number
    /YMULT=Y_Factor
    /YOFFSET=Y_Offset

SIMULATE  file_list
    /RANGE=(x_min,x_max)
    /RANGE
    /WEIGHT=(Wt_2,Wt_1,...Wt_n)
    /STEP=step_size
    /STEP
    /CAUCHY=(p_wid,p_ang)
    /CAUCHY
    /GAUSSIAN=(p_wid,p_ang)
    /GAUSSIAN
    /OFFSET=offset_val
```

```
    /AMORPHOUS=(a_wid,a_ang,a_int)
    /WAVELENGTH=wave_length
    /TARGET=target_type
    /TARGET
    /WTYPE=wave_type
    /NOISE=sig_level
    /NOISE
    /MAXIMUM=max_count
    /MAXIMUM

SUBTRACT
    /TITLE="file_title"
    /SCALE=scale_factor
    /OFFSET=offset_val
    /MINIMUM
    /IGNORE
    /CLIP

TITLE

WAVELENGTH  wave_length
    /TARGET=target_type
    /TARGET
    /NOTARGET
    /WTYPE=wave_type

WRITE  file_number
    /FILENAME=file_name
    /BINARY
    /NBS
    /PROFPV
    /GSAS
    /JONES
    /PEAKS
```

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